

FIGURE 1

**Amino acid sequence for full-length *E. faecalis* MvaS
with 6 residue polyhistidine C-terminal tag (tag is underlined)
[SEQ. ID No. 1]**

MTIGIDKISFFVPPYYIDMTALAEARNVDPGKFHIGIGQDQMAVNPISQDIVTFAANAAE
AILTKEDKEAIDMVIVGTESSIDESKAAAVVLHRLMGIQPFARSFEIKEACYGATAGLQL
AKNHVALHPDKKVLVVAADIAKYGLNSGGIPTQGAGAVAMLVASEPRILALKEDNVMLTQ
DIYDFWRPTGHPYPMVDGPLSNETYIQSFAQVWDEHKKRTGLDFADYDALAFHIPYTKMG
KKALLAKISDQTEAEQERILARYEESIVYSRRVGNLYTGSLYLGLISLLENATTLTAGNQ
IGLFSYGSGAVAEFFTGELVAGYQNHLQKETHLALLDNRTLSIAEYEAMFAETLDTDID
QTLEDELKYSISAINNTVRSYRNKGHHHHHH

FIGURE 1 (cont.)

cDNA sequence encoding MvaS
with 6 residue polyhistidine C-terminal tag (tag is underlined)
[SEQ. ID No. 2]

ATGACAATTGGGATTGATAAAATTAGTTTTTTTGTGCCCCCTTATTATATTGATATGACG
GCACTGGCTGAAGCCAGAAATGTAGACCCTGGAAAATTCATATTGGTATTGGGCAAGAC
CAAATGGCGGTGAACCCAATCAGCCAAGATATTGTGACATTTGCAGCCAATGCCGCAGAA
GCGATCTTGACCAAAGAAGATAAAGAGGCCATTGATATGGTGATTGTCGGGACTGAGTCC
AGTATCGATGAGTCAAAAAGCGCCGCAGTTGTCTTACATCGTTTAATGGGGATTCAACCT
TTCGCTCGCTCTTTCGAAATCAAGGAAGCTTGTTACGGAGCAACAGCAGGCTTACAGTTA
GCTAAGAATCACGTAGCCTTACATCCAGATAAAAAAGTCTTGGTCGTAGCGGCAGATATT
GCAAAATATGGCTTAAATTCTGGCGGTGAGCCTACACAAGGAGCTGGGGCGGTTGCAATG
TTAGTTGCTAGTGAACCGCGCATTTTGGCTTTTAAAAGAGGATAATGTGATGCTGACGCAA
GATATCTATGACTTTTGGCGTCCAACAGGCCACCCGTATCCTATGGTCGATGGTCCTTTG
TCAAACGAAACCTACATCCAATCTTTTGCCCAAGTCTGGGATGAACATAAAAAACGAACC
GGTCTTGATTTTGCAGATTATGATGCTTTAGCGTTCCATATTCCTTACACAAAAATGGGC
AAAAAGCCTTATTAGCAAAAATCTCCGACCAAACCTGAAGCAGAACAGGAACGAATTTTA
GCCCCGTTATGAAGAAAGTATCGTCTATAGTCGTCGCTAGGAAACTTGTATACGGGTTC
CTTTATCTGGGACTCATTTCCTTTTAGAAAATGCAACGACTTTAACCGCAGGCAATCAA
ATTGGTTTATTCAGTTATGGTTCTGGTGCTGTCGCTGAATTTTCACTGGTGAATTAGTA
GCTGGTTATCAAAATCATTTACAAAAGAACTCATTTAGCACTGCTGGATAATCGGACA
GAACTTTCTATCGCTGAATATGAAGCCATGTTTGCAGAACTTTAGACACAGACATTGAT
CAAACGTTAGAAGATGAATTAAAATATAGTATTTCTGCTATTAATAATACCGTTCGTTCT
TATCGAAACAAAGGGCCACCACCACCACCACCTAG

FIGURE 2

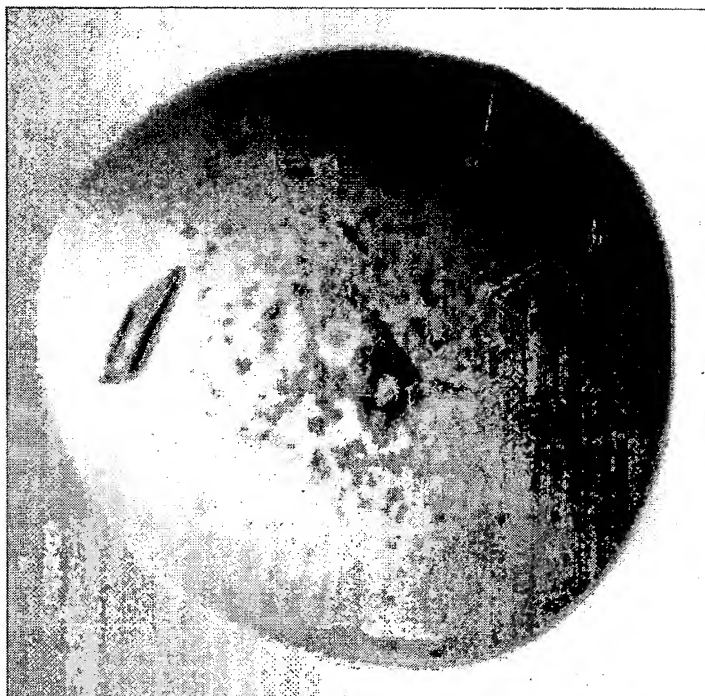


FIGURE 3

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	B	C	D	E	F	G	H	I	J
1	N	THR	A	2	54.202	21.266	59.185	1.00	12.76
3	CA	THR	A	2	53.298	22.012	58.259	1.00	12.73
5	CB	THR	A	2	53.265	21.336	56.877	1.00	12.92
7	OG1	THR	A	2	52.969	19.942	57.029	1.00	13.28
9	CG2	THR	A	2	54.644	21.356	56.213	1.00	13.54
13	C	THR	A	2	51.881	22.071	58.815	1.00	12.42
14	O	THR	A	2	51.505	21.269	59.663	1.00	12.26
17	N	ILE	A	3	51.110	23.043	58.334	1.00	12.20
19	CA	ILE	A	3	49.699	23.198	58.678	1.00	12.13
21	CB	ILE	A	3	49.512	24.327	59.734	1.00	12.36
23	CG1	ILE	A	3	50.240	23.994	61.046	1.00	13.14
26	CD1	ILE	A	3	50.999	25.158	61.613	1.00	14.29
30	CG2	ILE	A	3	48.031	24.568	60.020	1.00	12.57
34	C	ILE	A	3	48.939	23.545	57.398	1.00	11.73
35	O	ILE	A	3	49.438	24.307	56.575	1.00	11.68
36	N	GLY	A	4	47.738	23.004	57.224	1.00	11.36
38	CA	GLY	A	4	46.946	23.325	56.046	1.00	10.99
41	C	GLY	A	4	45.699	22.492	55.846	1.00	10.68
42	O	GLY	A	4	45.102	22.020	56.806	1.00	10.27
43	N	ILE	A	5	45.302	22.337	54.584	1.00	10.31
45	CA	ILE	A	5	44.117	21.575	54.219	1.00	10.15
47	CB	ILE	A	5	43.554	22.047	52.861	1.00	9.92
49	CG1	ILE	A	5	43.163	23.530	52.930	1.00	9.60
52	CD1	ILE	A	5	42.865	24.157	51.583	1.00	9.27
56	CG2	ILE	A	5	42.350	21.194	52.465	1.00	9.51
60	C	ILE	A	5	44.462	20.091	54.155	1.00	10.35
61	O	ILE	A	5	45.211	19.655	53.287	1.00	10.12
62	N	ASP	A	6	43.920	19.329	55.093	1.00	10.68
64	CA	ASP	A	6	44.139	17.891	55.151	1.00	11.01
66	CB	ASP	A	6	43.964	17.398	56.584	1.00	11.02
69	CG	ASP	A	6	44.307	15.939	56.733	1.00	11.04
70	OD1	ASP	A	6	43.452	15.165	57.209	1.00	11.93
71	OD2	ASP	A	6	45.403	15.477	56.377	1.00	11.09
72	C	ASP	A	6	43.167	17.151	54.235	1.00	11.30
73	O	ASP	A	6	43.541	16.204	53.543	1.00	11.21
74	N	LYS	A	7	41.912	17.583	54.264	1.00	11.57
76	CA	LYS	A	7	40.877	17.024	53.406	1.00	11.77
78	CB	LYS	A	7	40.084	15.959	54.161	1.00	11.90
81	CG	LYS	A	7	40.791	14.617	54.253	1.00	12.84
84	CD	LYS	A	7	39.941	13.586	54.991	1.00	13.41
87	CE	LYS	A	7	39.932	13.830	56.487	1.00	13.31
90	NZ	LYS	A	7	39.401	12.662	57.245	1.00	12.81
94	C	LYS	A	7	39.948	18.128	52.939	1.00	11.62

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
95	O	LYS	A	7	39.798	19.144	53.608	1.00	11.79
96	N	ILE	A	8	39.324	17.915	51.788	1.00	11.63
98	CA	ILE	A	8	38.470	18.916	51.167	1.00	11.75
100	CB	ILE	A	8	39.336	19.982	50.442	1.00	11.87
102	CG1	ILE	A	8	38.459	21.110	49.887	1.00	12.41
105	CD1	ILE	A	8	39.237	22.314	49.392	1.00	12.56
109	CG2	ILE	A	8	40.174	19.347	49.328	1.00	11.90
113	C	ILE	A	8	37.475	18.250	50.208	1.00	11.79
114	O	ILE	A	8	37.833	17.350	49.439	1.00	12.04
115	N	SER	A	9	36.221	18.688	50.281	1.00	11.37
117	CA	SER	A	9	35.157	18.175	49.424	1.00	11.02
119	CB	CSER	A	9	34.493	16.938	50.041	0.35	11.08
120	CB	BSER	A	9	34.474	16.996	50.111	0.65	11.31
125	OG	CSER	A	9	33.846	16.153	49.046	0.35	10.11
126	OG	BSER	A	9	33.959	17.399	51.375	0.65	11.90
129	C	SER	A	9	34.129	19.256	49.180	1.00	10.96
130	O	SER	A	9	34.100	20.268	49.879	1.00	10.68
131	N	PHE	A	10	33.282	19.045	48.183	1.00	10.54
133	CA	PHE	A	10	32.190	19.966	47.936	1.00	10.59
135	CB	PHE	A	10	32.477	20.855	46.715	1.00	10.51
138	CG	PHE	A	10	32.295	20.171	45.383	1.00	11.28
139	CD1	PHE	A	10	33.378	19.587	44.731	1.00	11.21
141	CE1	PHE	A	10	33.219	18.981	43.498	1.00	11.22
143	CZ	PHE	A	10	31.971	18.947	42.892	1.00	11.52
145	CE2	PHE	A	10	30.887	19.531	43.521	1.00	11.70
147	CD2	PHE	A	10	31.052	20.149	44.758	1.00	11.87
149	C	PHE	A	10	30.870	19.224	47.799	1.00	10.41
150	O	PHE	A	10	30.838	18.022	47.522	1.00	10.43
151	N	PHE	A	11	29.792	19.956	48.042	1.00	10.09
153	CA	PHE	A	11	28.441	19.477	47.811	1.00	10.04
155	CB	PHE	A	11	27.732	19.203	49.126	1.00	10.11
158	CG	PHE	A	11	26.362	18.629	48.953	1.00	10.84
159	CD1	PHE	A	11	26.194	17.278	48.696	1.00	11.42
161	CE1	PHE	A	11	24.920	16.739	48.525	1.00	11.03
163	CZ	PHE	A	11	23.813	17.554	48.603	1.00	10.90
165	CE2	PHE	A	11	23.968	18.907	48.854	1.00	11.21
167	CD2	PHE	A	11	25.237	19.442	49.022	1.00	10.79
169	C	PHE	A	11	27.669	20.527	47.033	1.00	9.94
170	O	PHE	A	11	27.855	21.723	47.243	1.00	9.62
171	N	VAL	A	12	26.818	20.063	46.123	1.00	9.67
173	CA	VAL	A	12	25.876	20.919	45.411	1.00	9.73
175	CB	VAL	A	12	26.335	21.192	43.950	1.00	9.74
177	CG1	VAL	A	12	27.651	21.953	43.945	1.00	9.55
181	CG2	VAL	A	12	26.466	19.894	43.145	1.00	9.78
185	C	VAL	A	12	24.511	20.228	45.433	1.00	9.88
186	O	VAL	A	12	24.442	19.008	45.587	1.00	9.71
187	N	PRO	A	13	23.429	20.990	45.295	1.00	10.22
188	CA	PRO	A	13	22.085	20.408	45.319	1.00	10.37
190	CB	PRO	A	13	21.176	21.637	45.234	1.00	10.35
193	CG	PRO	A	13	22.003	22.662	44.582	1.00	10.09
196	CD	PRO	A	13	23.381	22.450	45.106	1.00	10.13
199	C	PRO	A	13	21.840	19.462	44.138	1.00	10.73
200	O	PRO	A	13	22.529	19.556	43.129	1.00	10.40

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
201	N	PRO	A	14	20.867	18.566	44.268	1.00	11.46
202	CA	PRO	A	14	20.593	17.548	43.240	1.00	11.83
204	CB	PRO	A	14	19.724	16.531	43.991	1.00	11.99
207	CG	PRO	A	14	19.042	17.320	45.049	1.00	11.75
210	CD	PRO	A	14	19.976	18.430	45.432	1.00	11.49
213	C	PRO	A	14	19.868	18.031	41.974	1.00	12.30
214	O	PRO	A	14	19.307	17.189	41.277	1.00	12.17
215	N	TYR	A	15	19.876	19.333	41.684	1.00	12.69
217	CA	TYR	A	15	19.283	19.862	40.454	1.00	13.05
219	CB	TYR	A	15	17.974	20.597	40.764	1.00	13.30
222	CG	TYR	A	15	16.998	19.806	41.605	1.00	14.56
223	CD1	TYR	A	15	16.181	18.840	41.027	1.00	16.14
225	CE1	TYR	A	15	15.282	18.103	41.792	1.00	17.40
227	CZ	TYR	A	15	15.190	18.337	43.153	1.00	17.72
228	OH	TYR	A	15	14.299	17.606	43.904	1.00	18.77
230	CE2	TYR	A	15	15.990	19.295	43.753	1.00	17.03
232	CD2	TYR	A	15	16.888	20.025	42.975	1.00	16.32
234	C	TYR	A	15	20.222	20.821	39.717	1.00	12.88
235	O	TYR	A	15	21.107	21.430	40.311	1.00	12.42
236	N	TYR	A	16	20.009	20.942	38.412	1.00	12.94
238	CA	TYR	A	16	20.636	21.986	37.607	1.00	13.10
240	CB	TYR	A	16	21.992	21.519	37.079	1.00	13.06
243	CG	TYR	A	16	21.909	20.435	36.021	1.00	13.03
244	CD1	TYR	A	16	21.964	20.746	34.663	1.00	12.67
246	CE1	TYR	A	16	21.887	19.751	33.695	1.00	12.93
248	CZ	TYR	A	16	21.760	18.434	34.084	1.00	13.25
249	OH	TYR	A	16	21.685	17.437	33.140	1.00	14.53
251	CE2	TYR	A	16	21.707	18.101	35.423	1.00	13.25
253	CD2	TYR	A	16	21.779	19.098	36.380	1.00	12.97
255	C	TYR	A	16	19.746	22.354	36.427	1.00	13.45
256	O	TYR	A	16	18.871	21.582	36.048	1.00	13.46
257	N	ILE	A	17	19.977	23.531	35.852	1.00	13.65
259	CA	ILE	A	17	19.398	23.887	34.558	1.00	14.00
261	CB	ILE	A	17	18.515	25.177	34.624	1.00	14.14
263	CG1	ILE	A	17	17.841	25.419	33.261	1.00	14.75
266	CD1	ILE	A	17	16.856	26.590	33.213	1.00	15.47
270	CG2	ILE	A	17	19.330	26.410	35.028	1.00	14.31
274	C	ILE	A	17	20.531	24.041	33.548	1.00	14.08
275	O	ILE	A	17	21.597	24.582	33.864	1.00	13.99
276	N	ASP	A	18	20.300	23.535	32.342	1.00	14.02
278	CA	ASP	A	18	21.256	23.657	31.253	1.00	14.10
280	CB	ASP	A	18	20.886	22.694	30.127	1.00	14.36
283	CG	ASP	A	18	21.899	22.690	29.009	1.00	15.09
284	OD1	ASP	A	18	21.701	23.449	28.049	1.00	16.90
285	OD2	ASP	A	18	22.916	21.966	29.000	1.00	16.39
286	C	ASP	A	18	21.253	25.098	30.749	1.00	13.93
287	O	ASP	A	18	20.195	25.699	30.588	1.00	13.73
288	N	MSE	A	19	22.437	25.646	30.495	1.00	13.99
290	CA	MSE	A	19	22.571	27.055	30.129	1.00	14.18
292	CB	MSE	A	19	24.009	27.533	30.356	1.00	14.41
295	CG	MSE	A	19	24.431	27.530	31.835	1.00	14.83
298	SE	MSE	A	19	23.364	28.719	32.966	1.00	16.73
299	CE	MSE	A	19	24.021	30.366	32.299	1.00	14.28

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
303	C	MSE	A	19	22.108	27.366	28.696	1.00	14.36
304	O	MSE	A	19	21.753	28.510	28.399	1.00	14.04
305	N	THR	A	20	22.121	26.369	27.812	1.00	14.52
307	CA	THR	A	20	21.480	26.517	26.498	1.00	15.04
309	CB	THR	A	20	21.798	25.316	25.567	1.00	15.16
311	OG1	THR	A	20	23.183	25.341	25.202	1.00	15.54
313	CG2	THR	A	20	21.066	25.432	24.225	1.00	15.69
317	C	THR	A	20	19.975	26.684	26.682	1.00	15.04
318	O	THR	A	20	19.362	27.542	26.051	1.00	15.18
319	N	ALA	A	21	19.386	25.885	27.568	1.00	15.34
321	CA	ALA	A	21	17.953	25.981	27.857	1.00	15.33
323	CB	ALA	A	21	17.508	24.820	28.740	1.00	15.48
327	C	ALA	A	21	17.572	27.321	28.495	1.00	15.50
328	O	ALA	A	21	16.505	27.866	28.200	1.00	15.37
329	N	LEU	A	22	18.437	27.858	29.357	1.00	15.62
331	CA	LEU	A	22	18.184	29.161	29.975	1.00	15.90
333	CB	LEU	A	22	19.184	29.459	31.098	1.00	15.87
336	CG	LEU	A	22	18.985	30.800	31.816	1.00	15.98
338	CD1	LEU	A	22	17.648	30.831	32.550	1.00	16.60
342	CD2	LEU	A	22	20.133	31.088	32.774	1.00	16.14
346	C	LEU	A	22	18.262	30.259	28.921	1.00	16.25
347	O	LEU	A	22	17.420	31.147	28.883	1.00	15.88
348	N	ALA	A	23	19.280	30.180	28.069	1.00	16.78
350	CA	ALA	A	23	19.480	31.147	26.991	1.00	17.28
352	CB	ALA	A	23	20.737	30.798	26.196	1.00	17.30
356	C	ALA	A	23	18.265	31.206	26.069	1.00	17.81
357	O	ALA	A	23	17.804	32.287	25.719	1.00	17.89
358	N	GLU	A	24	17.737	30.042	25.702	1.00	18.41
360	CA	GLU	A	24	16.566	29.958	24.829	1.00	19.06
362	CB	GLU	A	24	16.231	28.494	24.513	1.00	19.40
365	CG	GLU	A	24	17.196	27.847	23.527	1.00	21.08
368	CD	GLU	A	24	17.045	26.335	23.425	1.00	23.42
369	OE1	GLU	A	24	17.752	25.719	22.590	1.00	24.83
370	OE2	GLU	A	24	16.231	25.753	24.176	1.00	25.56
371	C	GLU	A	24	15.363	30.666	25.453	1.00	19.03
372	O	GLU	A	24	14.706	31.466	24.798	1.00	19.00
373	N	ALA	A	25	15.102	30.388	26.728	1.00	19.06
375	CA	ALA	A	25	13.996	31.015	27.452	1.00	19.10
377	CB	ALA	A	25	13.843	30.383	28.826	1.00	19.13
381	C	ALA	A	25	14.171	32.531	27.588	1.00	19.09
382	O	ALA	A	25	13.185	33.274	27.601	1.00	18.96
383	N	ARG	A	26	15.424	32.977	27.671	1.00	19.04
385	CA	ARG	A	26	15.752	34.390	27.874	1.00	19.16
387	CB	ARG	A	26	17.009	34.514	28.744	1.00	18.89
390	CG	ARG	A	26	16.835	33.991	30.157	1.00	18.63
393	CD	ARG	A	26	16.147	34.961	31.102	1.00	18.00
396	NE	ARG	A	26	15.882	34.328	32.393	1.00	17.40
398	CZ	ARG	A	26	14.798	33.607	32.685	1.00	16.51
399	NH1	ARG	A	26	14.678	33.082	33.898	1.00	16.37
402	NH2	ARG	A	26	13.847	33.385	31.783	1.00	15.78
405	C	ARG	A	26	15.958	35.178	26.572	1.00	19.36
406	O	ARG	A	26	16.205	36.382	26.621	1.00	19.15
407	N	ASN	A	27	15.850	34.506	25.425	1.00	19.83

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
409	CA	ASN	A	27	16.103	35.119	24.116	1.00	20.28
411	CB	ASN	A	27	15.046	36.180	23.789	1.00	20.64
414	CG	ASN	A	27	13.636	35.648	23.897	1.00	21.76
415	OD1	ASN	A	27	13.253	34.723	23.177	1.00	23.63
416	ND2	ASN	A	27	12.849	36.230	24.800	1.00	24.44
419	C	ASN	A	27	17.507	35.715	24.030	1.00	20.29
420	O	ASN	A	27	17.695	36.851	23.590	1.00	20.27
421	N	VAL	A	28	18.481	34.918	24.459	1.00	20.19
423	CA	VAL	A	28	19.886	35.303	24.507	1.00	20.13
425	CB	VAL	A	28	20.348	35.416	25.986	1.00	20.20
427	CG1	VAL	A	28	21.867	35.474	26.113	1.00	20.44
431	CG2	VAL	A	28	19.715	36.633	26.636	1.00	20.75
435	C	VAL	A	28	20.698	34.244	23.764	1.00	19.93
436	O	VAL	A	28	20.304	33.078	23.719	1.00	19.72
437	N	ASP	A	29	21.817	34.648	23.168	1.00	19.84
439	CA	ASP	A	29	22.725	33.703	22.520	1.00	19.87
441	CB	ASP	A	29	23.974	34.403	21.995	1.00	20.36
444	CG	ASP	A	29	23.691	35.280	20.833	1.00	21.87
445	OD1	ASP	A	29	24.360	36.317	20.693	1.00	24.76
446	OD2	ASP	A	29	22.803	35.026	20.006	1.00	24.37
447	C	ASP	A	29	23.201	32.693	23.533	1.00	19.28
448	O	ASP	A	29	23.692	33.092	24.587	1.00	19.38
449	N	PRO	A	30	23.071	31.401	23.237	1.00	18.47
450	CA	PRO	A	30	23.710	30.376	24.068	1.00	18.01
452	CB	PRO	A	30	23.467	29.081	23.282	1.00	18.19
455	CG	PRO	A	30	22.258	29.351	22.464	1.00	18.39
458	CD	PRO	A	30	22.306	30.810	22.123	1.00	18.51
461	C	PRO	A	30	25.207	30.653	24.228	1.00	17.35
462	O	PRO	A	30	25.760	30.406	25.294	1.00	17.14
463	N	GLY	A	31	25.836	31.177	23.178	1.00	16.62
465	CA	GLY	A	31	27.241	31.541	23.206	1.00	16.12
468	C	GLY	A	31	27.595	32.624	24.213	1.00	15.61
469	O	GLY	A	31	28.709	32.647	24.707	1.00	15.49
470	N	LYS	A	32	26.671	33.533	24.512	1.00	15.15
472	CA	LYS	A	32	26.907	34.509	25.577	1.00	14.66
474	CB	LYS	A	32	25.757	35.512	25.714	1.00	14.83
477	CG	LYS	A	32	25.881	36.386	26.965	1.00	15.07
480	CD	LYS	A	32	25.019	37.630	26.928	1.00	15.92
483	CE	LYS	A	32	25.352	38.527	28.117	1.00	16.39
486	NZ	LYS	A	32	24.485	39.730	28.225	1.00	17.58
490	C	LYS	A	32	27.122	33.794	26.913	1.00	14.25
491	O	LYS	A	32	28.016	34.152	27.679	1.00	13.74
492	N	PHE	A	33	26.298	32.789	27.187	1.00	13.77
494	CA	PHE	A	33	26.402	32.045	28.437	1.00	13.51
496	CB	PHE	A	33	25.093	31.313	28.737	1.00	13.42
499	CG	PHE	A	33	23.943	32.224	29.113	1.00	13.19
500	CD1	PHE	A	33	24.128	33.589	29.342	1.00	13.57
502	CE1	PHE	A	33	23.058	34.404	29.686	1.00	12.97
504	CZ	PHE	A	33	21.796	33.870	29.807	1.00	13.22
506	CE2	PHE	A	33	21.597	32.517	29.593	1.00	13.79
508	CD2	PHE	A	33	22.666	31.704	29.244	1.00	13.39
510	C	PHE	A	33	27.580	31.068	28.449	1.00	13.45
511	O	PHE	A	33	28.331	31.040	29.413	1.00	13.33

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
512	N	HIS	A	34	27.740	30.285	27.384	1.00	13.16
514	CA	HIS	A	34	28.790	29.265	27.308	1.00	13.28
516	CB	AHIS	A	34	28.538	28.315	26.130	0.65	13.05
519	CG	AHIS	A	34	27.365	27.403	26.318	0.65	12.62
520	ND1A	HIS	A	34	27.336	26.415	27.278	0.65	11.69
522	CE1A	HIS	A	34	26.190	25.763	27.201	0.65	11.84
524	NE2A	HIS	A	34	25.473	26.293	26.227	0.65	11.89
526	CD2A	HIS	A	34	26.187	27.317	25.655	0.65	12.54
528	C	HIS	A	34	30.193	29.863	27.164	1.00	13.65
529	O	HIS	A	34	31.149	29.355	27.740	1.00	13.61
530	N	ILE	A	35	30.307	30.937	26.388	1.00	14.08
532	CA	ILE	A	35	31.606	31.508	26.039	1.00	14.54
534	CB	ILE	A	35	31.719	31.687	24.506	1.00	14.87
536	CG1	ILE	A	35	31.696	30.316	23.815	1.00	16.02
539	CD1	ILE	A	35	31.304	30.368	22.354	1.00	17.50
543	CG2	ILE	A	35	33.000	32.454	24.143	1.00	15.59
547	C	ILE	A	35	31.847	32.834	26.746	1.00	14.23
548	O	ILE	A	35	32.871	33.010	27.391	1.00	14.42
549	N	GLY	A	36	30.909	33.764	26.606	1.00	14.01
551	CA	GLY	A	36	31.053	35.099	27.155	1.00	13.69
554	C	GLY	A	36	31.202	35.137	28.666	1.00	13.42
555	O	GLY	A	36	32.059	35.849	29.193	1.00	13.42
556	N	ILE	A	37	30.372	34.362	29.354	1.00	12.85
558	CA	ILE	A	37	30.382	34.305	30.808	1.00	12.76
560	CB	ILE	A	37	28.936	34.356	31.348	1.00	12.91
562	CG1	ILE	A	37	28.347	35.751	31.086	1.00	13.62
565	CD1	ILE	A	37	26.855	35.841	31.283	1.00	14.41
569	CG2	ILE	A	37	28.891	34.047	32.835	1.00	13.07
573	C	ILE	A	37	31.142	33.059	31.265	1.00	12.16
574	O	ILE	A	37	31.944	33.134	32.187	1.00	11.96
575	N	GLY	A	38	30.884	31.925	30.614	1.00	11.77
577	CA	GLY	A	38	31.678	30.716	30.791	1.00	11.48
580	C	GLY	A	38	31.038	29.579	31.573	1.00	11.24
581	O	GLY	A	38	31.746	28.851	32.275	1.00	10.83
582	N	GLN	A	39	29.719	29.417	31.434	1.00	11.08
584	CA	GLN	A	39	28.939	28.431	32.187	1.00	11.05
586	CB	GLN	A	39	27.922	29.132	33.096	1.00	11.03
589	CG	GLN	A	39	28.463	30.262	33.959	1.00	10.92
592	CD	GLN	A	39	29.713	29.886	34.725	1.00	11.49
593	OE1	GLN	A	39	30.680	30.635	34.718	1.00	12.44
594	NE2	GLN	A	39	29.689	28.742	35.404	1.00	10.80
597	C	GLN	A	39	28.161	27.473	31.276	1.00	11.17
598	O	GLN	A	39	27.673	27.868	30.210	1.00	11.03
599	N	ASP	A	40	28.014	26.230	31.735	1.00	11.33
601	CA	ASP	A	40	27.286	25.180	31.006	1.00	11.34
603	CB	ASP	A	40	28.224	24.022	30.708	1.00	11.45
606	CG	ASP	A	40	29.402	24.445	29.875	1.00	11.30
607	OD1	ASP	A	40	30.514	23.932	30.118	1.00	11.57
608	OD2	ASP	A	40	29.300	25.294	28.963	1.00	11.08
609	C	ASP	A	40	26.063	24.649	31.751	1.00	11.49
610	O	ASP	A	40	25.033	24.376	31.136	1.00	11.09
611	N	GLN	A	41	26.197	24.473	33.065	1.00	11.59
613	CA	GLN	A	41	25.106	24.023	33.927	1.00	11.82

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
615	CB	GLN	A	41	25.240	22.520	34.241	1.00	12.05
618	CG	GLN	A	41	25.568	21.618	33.021	1.00	13.21
621	CD	GLN	A	41	25.873	20.161	33.394	1.00	14.52
622	OE1	GLN	A	41	26.563	19.891	34.379	1.00	13.91
623	NE2	GLN	A	41	25.366	19.225	32.593	1.00	16.25
626	C	GLN	A	41	25.131	24.846	35.222	1.00	11.84
627	O	GLN	A	41	26.204	25.125	35.755	1.00	11.66
628	N	MSE	A	42	23.950	25.228	35.710	1.00	11.86
630	CA	MSE	A	42	23.792	26.025	36.929	1.00	12.11
632	CB	MSE	A	42	22.932	27.260	36.643	1.00	12.54
635	CG	MSE	A	42	22.262	27.873	37.893	1.00	14.05
638	SE	MSE	A	42	20.813	29.094	37.490	1.00	17.99
639	CE	MSE	A	42	21.767	30.128	36.184	1.00	13.71
643	C	MSE	A	42	23.118	25.205	38.030	1.00	11.66
644	O	MSE	A	42	22.049	24.647	37.814	1.00	11.88
645	N	ALA	A	43	23.719	25.179	39.215	1.00	11.19
647	CA	ALA	A	43	23.119	24.533	40.381	1.00	10.83
649	CB	ALA	A	43	24.126	24.455	41.516	1.00	10.95
653	C	ALA	A	43	21.876	25.300	40.833	1.00	10.69
654	O	ALA	A	43	21.878	26.532	40.867	1.00	10.31
655	N	VAL	A	44	20.822	24.558	41.162	1.00	10.31
657	CA	VAL	A	44	19.573	25.124	41.679	1.00	10.37
659	CB	AVAL	A	44	18.457	25.128	40.607	0.65	10.06
661	CG1AVAL	A	44	17.245	25.923	41.090	0.65	10.02	
665	CG2AVAL	A	44	18.973	25.693	39.290	0.65	10.22	
669	C	VAL	A	44	19.109	24.287	42.871	1.00	10.47
670	O	VAL	A	44	19.283	23.067	42.876	1.00	10.39
671	N	ASN	A	45	18.525	24.947	43.874	1.00	10.73
673	CA	ASN	A	45	18.023	24.271	45.075	1.00	10.88
675	CB	ASN	A	45	18.976	24.481	46.255	1.00	11.00
678	CG	ASN	A	45	19.019	25.925	46.730	1.00	11.03
679	OD1	ASN	A	45	19.650	26.778	46.103	1.00	12.28
680	ND2	ASN	A	45	18.349	26.204	47.846	1.00	10.36
683	C	ASN	A	45	16.622	24.741	45.471	1.00	10.98
684	O	ASN	A	45	16.277	25.909	45.274	1.00	10.93
685	N	PRO	A	46	15.819	23.839	46.037	1.00	11.03
686	CA	PRO	A	46	14.504	24.216	46.561	1.00	11.13
688	CB	PRO	A	46	13.773	22.875	46.652	1.00	11.07
691	CG	PRO	A	46	14.862	21.894	46.968	1.00	11.32
694	CD	PRO	A	46	16.086	22.402	46.229	1.00	11.02
697	C	PRO	A	46	14.625	24.859	47.940	1.00	11.19
698	O	PRO	A	46	15.711	24.844	48.540	1.00	11.08
699	N	ILE	A	47	13.512	25.398	48.434	1.00	11.09
701	CA	ILE	A	47	13.465	26.082	49.731	1.00	11.17
703	CB	ILE	A	47	12.114	26.833	49.909	1.00	11.38
705	CG1	ILE	A	47	10.924	25.922	49.562	1.00	12.55
708	CD1	ILE	A	47	9.662	26.210	50.348	1.00	13.79
712	CG2	ILE	A	47	12.095	28.069	49.058	1.00	12.16
716	C	ILE	A	47	13.692	25.144	50.920	1.00	10.64
717	O	ILE	A	47	13.913	25.603	52.038	1.00	10.56
718	N	SER	A	48	13.629	23.835	50.673	1.00	10.28
720	CA	SER	A	48	13.890	22.828	51.699	1.00	9.93
722	CB	SER	A	48	13.142	21.531	51.370	1.00	9.94

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
725	OG	SER	A	48	13.407	21.104	50.045	1.00	9.71
727	C	SER	A	48	15.381	22.529	51.896	1.00	9.68
728	O	SER	A	48	15.736	21.669	52.702	1.00	9.62
729	N	GLN	A	49	16.249	23.230	51.167	1.00	9.36
731	CA	GLN	A	49	17.699	23.087	51.316	1.00	8.98
733	CB	GLN	A	49	18.290	22.411	50.078	1.00	8.84
736	CG	GLN	A	49	17.717	21.006	49.829	1.00	8.93
739	CD	GLN	A	49	18.158	20.390	48.512	1.00	8.85
740	OE1	GLN	A	49	19.162	20.803	47.919	1.00	8.61
741	NE2	GLN	A	49	17.403	19.395	48.048	1.00	8.11
744	C	GLN	A	49	18.336	24.458	51.550	1.00	8.87
745	O	GLN	A	49	18.130	25.382	50.761	1.00	8.42
746	N	ASP	A	50	19.087	24.582	52.648	1.00	8.68
748	CA	ASP	A	50	19.737	25.835	53.030	1.00	8.68
750	CB	ASP	A	50	19.026	26.463	54.248	1.00	8.61
753	CG	ASP	A	50	19.161	25.627	55.517	1.00	9.06
754	OD1	ASP	A	50	18.396	25.864	56.473	1.00	9.22
755	OD2	ASP	A	50	19.990	24.714	55.662	1.00	8.75
756	C	ASP	A	50	21.233	25.596	53.282	1.00	8.79
757	O	ASP	A	50	21.743	24.511	52.994	1.00	8.31
758	N	ILE	A	51	21.942	26.599	53.796	1.00	8.88
760	CA	ILE	A	51	23.389	26.471	53.992	1.00	9.16
762	CB	ILE	A	51	24.049	27.815	54.403	1.00	9.22
764	CG1	ILE	A	51	23.437	28.382	55.688	1.00	9.46
767	CD1	ILE	A	51	24.332	29.393	56.375	1.00	10.27
771	CG2	ILE	A	51	23.962	28.831	53.254	1.00	9.17
775	C	ILE	A	51	23.772	25.365	54.976	1.00	9.27
776	O	ILE	A	51	24.843	24.780	54.854	1.00	9.30
777	N	VAL	A	52	22.915	25.094	55.955	1.00	9.36
779	CA	VAL	A	52	23.147	23.980	56.875	1.00	9.56
781	CB	VAL	A	52	22.164	24.013	58.072	1.00	9.60
783	CG1	VAL	A	52	22.227	22.726	58.887	1.00	10.02
787	CG2	VAL	A	52	22.451	25.216	58.957	1.00	9.30
791	C	VAL	A	52	23.069	22.641	56.125	1.00	9.53
792	O	VAL	A	52	23.895	21.762	56.339	1.00	9.54
793	N	THR	A	53	22.073	22.492	55.259	1.00	9.66
795	CA	THR	A	53	21.955	21.306	54.405	1.00	9.55
797	CB	THR	A	53	20.789	21.480	53.406	1.00	9.50
799	OG1	THR	A	53	19.553	21.663	54.115	1.00	8.91
801	CG2	THR	A	53	20.580	20.212	52.565	1.00	9.74
805	C	THR	A	53	23.236	21.047	53.619	1.00	9.49
806	O	THR	A	53	23.761	19.933	53.619	1.00	9.29
807	N	PHE	A	54	23.730	22.081	52.944	1.00	9.46
809	CA	PHE	A	54	24.903	21.941	52.086	1.00	9.60
811	CB	PHE	A	54	25.073	23.180	51.196	1.00	9.77
814	CG	PHE	A	54	23.902	23.451	50.275	1.00	10.24
815	CD1	PHE	A	54	23.664	24.737	49.818	1.00	11.07
817	CE1	PHE	A	54	22.602	25.006	48.969	1.00	11.79
819	CZ	PHE	A	54	21.764	23.983	48.567	1.00	11.82
821	CE2	PHE	A	54	21.987	22.695	49.008	1.00	11.72
823	CD2	PHE	A	54	23.051	22.429	49.856	1.00	11.25
825	C	PHE	A	54	26.167	21.703	52.907	1.00	9.52
826	O	PHE	A	54	26.993	20.870	52.545	1.00	9.43

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
827	N	ALA	A	55	26.308	22.436	54.009	1.00	9.48
829	CA	ALA	A	55	27.489	22.343	54.863	1.00	9.61
831	CB	ALA	A	55	27.458	23.426	55.938	1.00	9.73
835	C	ALA	A	55	27.603	20.965	55.507	1.00	9.72
836	O	ALA	A	55	28.687	20.396	55.558	1.00	9.74
837	N	ALA	A	56	26.478	20.428	55.972	1.00	9.72
839	CA	ALA	A	56	26.451	19.111	56.611	1.00	9.90
841	CB	ALA	A	56	25.085	18.849	57.223	1.00	9.91
845	C	ALA	A	56	26.809	17.999	55.617	1.00	9.86
846	O	ALA	A	56	27.559	17.089	55.946	1.00	10.08
847	N	ASN	A	57	26.282	18.084	54.402	1.00	9.75
849	CA	ASN	A	57	26.573	17.082	53.377	1.00	10.16
851	CB	ASN	A	57	25.614	17.227	52.186	1.00	9.90
854	CG	ASN	A	57	24.273	16.544	52.432	1.00	10.88
855	OD1	ASN	A	57	24.200	15.315	52.494	1.00	11.08
856	ND2	ASN	A	57	23.208	17.339	52.591	1.00	9.43
859	C	ASN	A	57	28.042	17.128	52.931	1.00	10.26
860	O	ASN	A	57	28.675	16.086	52.753	1.00	10.39
861	N	ALA	A	58	28.592	18.332	52.804	1.00	10.35
863	CA	ALA	A	58	29.985	18.501	52.397	1.00	10.70
865	CB	ALA	A	58	30.264	19.955	52.072	1.00	10.67
869	C	ALA	A	58	30.950	17.997	53.477	1.00	10.99
870	O	ALA	A	58	31.872	17.237	53.187	1.00	10.93
871	N	ALA	A	59	30.706	18.411	54.715	1.00	11.42
873	CA	ALA	A	59	31.533	18.040	55.859	1.00	11.86
875	CB	ALA	A	59	31.074	18.799	57.100	1.00	11.98
879	C	ALA	A	59	31.502	16.536	56.126	1.00	12.44
880	O	ALA	A	59	32.529	15.936	56.446	1.00	12.41
881	N	GLU	A	60	30.327	15.932	55.985	1.00	12.73
883	CA	GLU	A	60	30.156	14.499	56.220	1.00	13.31
885	CB	GLU	A	60	28.690	14.110	56.046	1.00	13.48
888	CG	GLU	A	60	28.414	12.641	56.303	1.00	14.88
891	CD	GLU	A	60	26.964	12.388	56.630	1.00	15.94
892	OE1	GLU	A	60	26.614	12.446	57.824	1.00	16.74
893	OE2	GLU	A	60	26.183	12.153	55.690	1.00	16.79
894	C	GLU	A	60	31.032	13.638	55.301	1.00	13.32
895	O	GLU	A	60	31.443	12.540	55.683	1.00	13.40
896	N	ALA	A	61	31.318	14.140	54.101	1.00	13.39
898	CA	ALA	A	61	32.189	13.448	53.148	1.00	13.61
900	CB	ALA	A	61	32.114	14.127	51.777	1.00	13.57
904	C	ALA	A	61	33.658	13.336	53.593	1.00	13.74
905	O	ALA	A	61	34.402	12.523	53.042	1.00	13.86
906	N	ILE	A	62	34.078	14.141	54.571	1.00	13.64
908	CA	ILE	A	62	35.483	14.170	54.988	1.00	13.81
910	CB	ILE	A	62	36.138	15.528	54.611	1.00	13.73
912	CG1	ILE	A	62	35.407	16.704	55.272	1.00	13.83
915	CD1	ILE	A	62	36.198	17.998	55.266	1.00	13.82
919	CG2	ILE	A	62	36.173	15.701	53.090	1.00	14.19
923	C	ILE	A	62	35.754	13.868	56.470	1.00	13.93
924	O	ILE	A	62	36.914	13.738	56.848	1.00	14.43
925	N	LEU	A	63	34.722	13.756	57.307	1.00	13.93
927	CA	LEU	A	63	34.937	13.626	58.754	1.00	14.10
929	CB	LEU	A	63	33.939	14.490	59.528	1.00	14.11

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
932	CG	LEU	A	63	34.000	16.011	59.349	1.00	14.11
934	CD1	LEU	A	63	33.078	16.666	60.355	1.00	14.85
938	CD2	LEU	A	63	35.412	16.564	59.478	1.00	13.81
942	C	LEU	A	63	34.853	12.185	59.273	1.00	14.48
943	O	LEU	A	63	33.834	11.515	59.108	1.00	14.48
944	N	THR	A	64	35.928	11.737	59.920	1.00	14.71
946	CA	THR	A	64	35.965	10.453	60.612	1.00	14.96
948	CB	THR	A	64	37.362	9.816	60.521	1.00	14.98
950	OG1	THR	A	64	38.322	10.652	61.184	1.00	13.73
952	CG2	THR	A	64	37.858	9.734	59.068	1.00	15.18
956	C	THR	A	64	35.625	10.688	62.077	1.00	15.39
957	O	THR	A	64	35.547	11.830	62.524	1.00	15.05
958	N	LYS	A	65	35.455	9.607	62.828	1.00	15.85
960	CA	LYS	A	65	35.156	9.708	64.254	1.00	16.51
962	CB	LYS	A	65	34.752	8.343	64.838	1.00	16.93
965	CG	LYS	A	65	35.879	7.432	65.303	1.00	19.15
968	CD	LYS	A	65	35.328	6.281	66.159	1.00	21.61
971	CE	LYS	A	65	35.187	6.694	67.630	1.00	23.10
974	NZ	LYS	A	65	34.275	5.798	68.409	1.00	23.96
978	C	LYS	A	65	36.324	10.341	65.013	1.00	16.23
979	O	LYS	A	65	36.121	11.066	65.981	1.00	16.07
980	N	GLU	A	66	37.539	10.091	64.537	1.00	16.15
982	CA	GLU	A	66	38.743	10.654	65.139	1.00	16.18
984	CB	GLU	A	66	39.998	9.974	64.577	1.00	16.57
987	CG	GLU	A	66	40.201	8.527	65.026	1.00	17.97
990	CD	GLU	A	66	39.331	7.518	64.283	1.00	20.11
991	OE1	GLU	A	66	38.981	6.482	64.895	1.00	21.72
992	OE2	GLU	A	66	38.994	7.743	63.095	1.00	20.15
993	C	GLU	A	66	38.804	12.169	64.898	1.00	15.55
994	O	GLU	A	66	39.147	12.930	65.795	1.00	15.36
995	N	ASP	A	67	38.464	12.596	63.684	1.00	15.02
997	CA	ASP	A	67	38.398	14.021	63.358	1.00	14.45
999	CB	ASP	A	67	37.952	14.241	61.909	1.00	14.27
1002	CG	ASP	A	67	38.970	13.761	60.892	1.00	14.31
1003	OD1	ASP	A	67	38.549	13.401	59.771	1.00	13.66
1004	OD2	ASP	A	67	40.199	13.715	61.111	1.00	13.56
1005	C	ASP	A	67	37.423	14.738	64.290	1.00	14.17
1006	O	ASP	A	67	37.713	15.823	64.780	1.00	13.76
1007	N	LYS	A	68	36.273	14.117	64.533	1.00	14.15
1009	CA	LYS	A	68	35.216	14.714	65.349	1.00	14.43
1011	CB	LYS	A	68	33.941	13.858	65.289	1.00	14.38
1014	CG	LYS	A	68	33.270	13.844	63.921	1.00	14.69
1017	CD	LYS	A	68	32.285	12.687	63.772	1.00	14.89
1020	CE	LYS	A	68	31.688	12.645	62.372	1.00	15.19
1023	NZ	LYS	A	68	30.360	11.982	62.339	1.00	15.93
1027	C	LYS	A	68	35.645	14.932	66.805	1.00	14.61
1028	O	LYS	A	68	35.166	15.859	67.453	1.00	14.84
1029	N	GLU	A	69	36.539	14.089	67.318	1.00	14.70
1031	CA	GLU	A	69	37.087	14.285	68.667	1.00	14.91
1033	CB	GLU	A	69	37.578	12.957	69.261	1.00	15.31
1036	CG	GLU	A	69	36.508	11.886	69.435	1.00	17.18
1039	CD	GLU	A	69	35.369	12.297	70.360	1.00	19.72
1040	OE1	GLU	A	69	34.204	11.955	70.050	1.00	21.65

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1041	OE2	GLU	A	69	35.627	12.956	71.391	1.00	20.78
1042	C	GLU	A	69	38.236	15.305	68.689	1.00	14.33
1043	O	GLU	A	69	38.487	15.933	69.710	1.00	14.23
1044	N	ALA	A	70	38.937	15.459	67.569	1.00	13.75
1046	CA	ALA	A	70	40.089	16.361	67.497	1.00	13.33
1048	CB	ALA	A	70	41.101	15.833	66.492	1.00	13.40
1052	C	ALA	A	70	39.710	17.807	67.151	1.00	12.66
1053	O	ALA	A	70	40.496	18.724	67.391	1.00	12.47
1054	N	ILE	A	71	38.518	18.008	66.591	1.00	11.85
1056	CA	ILE	A	71	38.064	19.344	66.211	1.00	11.47
1058	CB	ILE	A	71	36.931	19.275	65.163	1.00	11.36
1060	CG1	ILE	A	71	37.465	18.779	63.817	1.00	11.45
1063	CD1	ILE	A	71	36.378	18.256	62.888	1.00	11.32
1067	CG2	ILE	A	71	36.281	20.652	64.970	1.00	11.31
1071	C	ILE	A	71	37.579	20.107	67.442	1.00	10.92
1072	O	ILE	A	71	36.707	19.639	68.168	1.00	10.81
1073	N	ASP	A	72	38.148	21.283	67.673	1.00	10.67
1075	CA	ASP	A	72	37.672	22.159	68.738	1.00	10.44
1077	CB	ASP	A	72	38.694	22.224	69.880	1.00	10.61
1080	CG	ASP	A	72	39.945	23.004	69.518	1.00	10.78
1081	OD1	ASP	A	72	40.183	23.276	68.321	1.00	10.77
1082	OD2	ASP	A	72	40.755	23.383	70.384	1.00	11.55
1083	C	ASP	A	72	37.295	23.559	68.231	1.00	10.25
1084	O	ASP	A	72	37.127	24.479	69.024	1.00	10.14
1085	N	MSE	A	73	37.177	23.712	66.915	1.00	9.93
1087	CA	MSE	A	73	36.603	24.918	66.321	1.00	9.92
1089	CB	MSE	A	73	37.672	25.990	66.073	1.00	10.02
1092	CG	MSE	A	73	37.094	27.346	65.653	1.00	11.07
1095	SE	MSE	A	73	38.335	28.847	65.896	1.00	13.87
1096	CE	MSE	A	73	39.739	28.213	64.801	1.00	12.03
1100	C	MSE	A	73	35.880	24.579	65.022	1.00	9.47
1101	O	MSE	A	73	36.356	23.776	64.222	1.00	9.43
1102	N	VAL	A	74	34.718	25.194	64.839	1.00	9.21
1104	CA	VAL	A	74	33.873	24.994	63.671	1.00	9.07
1106	CB	VAL	A	74	32.604	24.184	64.030	1.00	9.03
1108	CG1	VAL	A	74	31.704	23.991	62.809	1.00	8.94
1112	CG2	VAL	A	74	32.985	22.839	64.633	1.00	9.27
1116	C	VAL	A	74	33.476	26.378	63.151	1.00	8.82
1117	O	VAL	A	74	32.859	27.159	63.873	1.00	8.43
1118	N	ILE	A	75	33.847	26.673	61.907	1.00	8.63
1120	CA	ILE	A	75	33.570	27.966	61.287	1.00	8.56
1122	CB	ILE	A	75	34.886	28.698	60.947	1.00	8.55
1124	CG1	ILE	A	75	35.773	28.833	62.187	1.00	8.60
1127	CD1	ILE	A	75	37.127	29.466	61.912	1.00	8.51
1131	CG2	ILE	A	75	34.594	30.077	60.346	1.00	8.56
1135	C	ILE	A	75	32.773	27.751	60.013	1.00	8.34
1136	O	ILE	A	75	33.154	26.939	59.179	1.00	8.41
1137	N	VAL	A	76	31.667	28.471	59.869	1.00	8.30
1139	CA	VAL	A	76	30.967	28.560	58.590	1.00	8.31
1141	CB	VAL	A	76	29.468	28.232	58.724	1.00	8.34
1143	CG1	VAL	A	76	28.712	28.535	57.424	1.00	8.39
1147	CG2	VAL	A	76	29.282	26.776	59.111	1.00	8.97
1151	C	VAL	A	76	31.141	29.973	58.053	1.00	8.09

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1152	O	VAL	A	76	30.773	30.936	58.719	1.00	8.06
1153	N	GLY	A	77	31.735	30.087	56.867	1.00	8.02
1155	CA	GLY	A	77	31.753	31.328	56.113	1.00	7.89
1158	C	GLY	A	77	30.579	31.370	55.148	1.00	7.71
1159	O	GLY	A	77	30.398	30.463	54.332	1.00	7.60
1160	N	THR	A	78	29.777	32.421	55.242	1.00	7.48
1162	CA	THR	A	78	28.583	32.553	54.416	1.00	7.39
1164	CB	THR	A	78	27.446	31.655	54.997	1.00	7.27
1166	OG1	THR	A	78	26.329	31.596	54.096	1.00	6.69
1168	CG2	THR	A	78	26.874	32.236	56.282	1.00	7.23
1172	C	THR	A	78	28.124	34.008	54.312	1.00	7.62
1173	O	THR	A	78	28.470	34.849	55.145	1.00	8.02
1174	N	GLU	A	79	27.376	34.289	53.254	1.00	7.72
1176	CA	GLU	A	79	26.596	35.514	53.114	1.00	7.58
1178	CB	GLU	A	79	27.162	36.384	51.981	1.00	7.61
1181	CG	GLU	A	79	27.153	35.719	50.614	1.00	7.60
1184	CD	GLU	A	79	27.605	36.653	49.510	1.00	7.88
1185	OE1	GLU	A	79	26.772	37.432	49.009	1.00	8.45
1186	OE2	GLU	A	79	28.795	36.608	49.149	1.00	7.55
1187	C	GLU	A	79	25.130	35.170	52.833	1.00	7.49
1188	O	GLU	A	79	24.377	36.019	52.374	1.00	7.22
1189	N	SER	A	80	24.740	33.923	53.112	1.00	7.54
1191	CA	SER	A	80	23.378	33.431	52.882	1.00	7.58
1193	CB	SER	A	80	23.405	32.279	51.875	1.00	7.71
1196	OG	SER	A	80	23.947	32.697	50.639	1.00	7.17
1198	C	SER	A	80	22.756	32.949	54.193	1.00	7.76
1199	O	SER	A	80	22.122	31.889	54.248	1.00	7.40
1200	N	SER	A	81	22.933	33.738	55.249	1.00	7.78
1202	CA	SER	A	81	22.553	33.312	56.593	1.00	7.91
1204	CB	SER	A	81	23.118	34.271	57.647	1.00	7.95
1207	OG	SER	A	81	22.560	35.566	57.524	1.00	6.84
1209	C	SER	A	81	21.039	33.192	56.761	1.00	8.38
1210	O	SER	A	81	20.271	33.825	56.043	1.00	8.26
1211	N	ILE	A	82	20.636	32.365	57.722	1.00	8.89
1213	CA	ILE	A	82	19.230	32.152	58.070	1.00	9.25
1215	CB	ILE	A	82	18.861	30.654	57.923	1.00	9.41
1217	CG1	ILE	A	82	19.725	29.776	58.839	1.00	10.65
1220	CD1	ILE	A	82	19.475	28.291	58.698	1.00	11.86
1224	CG2	ILE	A	82	19.014	30.235	56.459	1.00	10.24
1228	C	ILE	A	82	18.892	32.662	59.468	1.00	9.16
1229	O	ILE	A	82	17.729	32.639	59.881	1.00	9.55
1230	N	ASP	A	83	19.907	33.127	60.189	1.00	8.91
1232	CA	ASP	A	83	19.713	33.773	61.478	1.00	8.84
1234	CB	ASP	A	83	19.922	32.767	62.617	1.00	8.51
1237	CG	ASP	A	83	19.138	33.126	63.865	1.00	8.43
1238	OD1	ASP	A	83	18.029	32.587	64.073	1.00	7.70
1239	OD2	ASP	A	83	19.558	33.944	64.699	1.00	6.58
1240	C	ASP	A	83	20.676	34.953	61.614	1.00	8.75
1241	O	ASP	A	83	21.805	34.910	61.115	1.00	9.10
1242	N	GLU	A	84	20.219	36.008	62.282	1.00	8.77
1244	CA	GLU	A	84	21.024	37.213	62.496	1.00	8.82
1246	CB	GLU	A	84	20.120	38.441	62.640	1.00	8.81
1249	CG	GLU	A	84	19.238	38.735	61.438	1.00	9.44

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1252	CD	GLU	A	84	20.022	39.129	60.197	1.00	9.80
1253	OE1	GLU	A	84	21.181	39.586	60.331	1.00	8.70
1254	OE2	GLU	A	84	19.465	38.973	59.086	1.00	9.67
1255	C	GLU	A	84	21.906	37.113	63.741	1.00	8.57
1256	O	GLU	A	84	22.822	37.920	63.916	1.00	8.58
1257	N	SER	A	85	21.608	36.146	64.609	1.00	8.36
1259	CA	SER	A	85	22.339	35.948	65.864	1.00	8.05
1261	CB	SER	A	85	21.383	36.080	67.054	1.00	8.08
1264	OG	SER	A	85	21.993	35.694	68.274	1.00	7.24
1266	C	SER	A	85	23.034	34.589	65.924	1.00	8.01
1267	O	SER	A	85	24.230	34.520	66.163	1.00	8.24
1268	N	LYS	A	86	22.273	33.515	65.728	1.00	8.08
1270	CA	LYS	A	86	22.772	32.150	65.913	1.00	7.68
1272	CB	LYS	A	86	21.603	31.192	66.152	1.00	7.76
1275	CG	LYS	A	86	22.005	29.734	66.397	1.00	7.63
1278	CD	LYS	A	86	20.839	28.937	66.967	1.00	7.97
1281	CE	LYS	A	86	21.142	27.444	67.027	1.00	8.16
1284	NZ	LYS	A	86	20.401	26.760	68.125	1.00	8.15
1288	C	LYS	A	86	23.583	31.684	64.707	1.00	7.48
1289	O	LYS	A	86	23.070	31.612	63.591	1.00	7.15
1290	N	ALA	A	87	24.848	31.347	64.947	1.00	7.38
1292	CA	ALA	A	87	25.752	30.927	63.888	1.00	7.23
1294	CB	ALA	A	87	27.168	30.802	64.420	1.00	7.23
1298	C	ALA	A	87	25.296	29.601	63.299	1.00	7.30
1299	O	ALA	A	87	24.928	28.681	64.034	1.00	6.89
1300	N	ALA	A	88	25.315	29.521	61.968	1.00	7.54
1302	CA	ALA	A	88	25.046	28.280	61.251	1.00	7.62
1304	CB	ALA	A	88	25.209	28.496	59.756	1.00	7.62
1308	C	ALA	A	88	25.978	27.167	61.731	1.00	7.54
1309	O	ALA	A	88	25.605	26.003	61.729	1.00	7.60
1310	N	ALA	A	89	27.187	27.541	62.139	1.00	7.81
1312	CA	ALA	A	89	28.183	26.593	62.642	1.00	7.82
1314	CB	ALA	A	89	29.474	27.322	62.972	1.00	7.91
1318	C	ALA	A	89	27.712	25.800	63.861	1.00	8.06
1319	O	ALA	A	89	28.165	24.681	64.079	1.00	7.82
1320	N	VAL	A	90	26.821	26.380	64.660	1.00	8.22
1322	CA	VAL	A	90	26.307	25.699	65.846	1.00	8.77
1324	CB	VAL	A	90	25.449	26.638	66.736	1.00	8.77
1326	CG1	VAL	A	90	24.844	25.871	67.894	1.00	9.00
1330	CG2	VAL	A	90	26.291	27.799	67.244	1.00	8.82
1334	C	VAL	A	90	25.487	24.472	65.459	1.00	9.04
1335	O	VAL	A	90	25.661	23.402	66.036	1.00	8.95
1336	N	VAL	A	91	24.595	24.626	64.485	1.00	9.29
1338	CA	VAL	A	91	23.777	23.505	64.032	1.00	9.56
1340	CB	VAL	A	91	22.641	23.954	63.095	1.00	9.78
1342	CG1	VAL	A	91	21.824	22.753	62.625	1.00	9.69
1346	CG2	VAL	A	91	21.739	24.972	63.801	1.00	10.13
1350	C	VAL	A	91	24.658	22.465	63.338	1.00	9.53
1351	O	VAL	A	91	24.468	21.264	63.527	1.00	9.69
1352	N	LEU	A	92	25.622	22.936	62.546	1.00	9.56
1354	CA	LEU	A	92	26.579	22.061	61.876	1.00	9.52
1356	CB	LEU	A	92	27.537	22.876	60.993	1.00	9.63
1359	CG	LEU	A	92	28.615	22.092	60.236	1.00	9.79

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1361	CD1	LEU	A	92	27.985	21.088	59.288	1.00	9.95
1365	CD2	LEU	A	92	29.537	23.039	59.479	1.00	10.31
1369	C	LEU	A	92	27.372	21.236	62.890	1.00	9.42
1370	O	LEU	A	92	27.619	20.052	62.666	1.00	9.26
1371	N	HIS	A	93	27.751	21.861	64.004	1.00	9.42
1373	CA	HIS	A	93	28.475	21.182	65.085	1.00	9.52
1375	CB	HIS	A	93	28.813	22.168	66.218	1.00	9.54
1378	CG	HIS	A	93	29.417	21.525	67.433	1.00	9.46
1379	ND1	HIS	A	93	28.662	20.890	68.398	1.00	9.46
1381	CE1	HIS	A	93	29.460	20.419	69.340	1.00	9.30
1383	NE2	HIS	A	93	30.703	20.741	69.031	1.00	8.60
1385	CD2	HIS	A	93	30.704	21.431	67.843	1.00	8.77
1387	C	HIS	A	93	27.672	19.988	65.623	1.00	9.52
1388	O	HIS	A	93	28.234	18.914	65.831	1.00	9.62
1389	N	ARG	A	94	26.368	20.178	65.837	1.00	9.50
1391	CA	ARG	A	94	25.491	19.098	66.312	1.00	9.69
1393	CB	ARG	A	94	24.086	19.616	66.668	1.00	9.81
1396	CG	ARG	A	94	23.074	18.492	67.003	1.00	9.95
1399	CD	ARG	A	94	21.692	18.955	67.454	1.00	10.32
1402	NE	ARG	A	94	20.960	19.637	66.388	1.00	10.94
1404	CZ	ARG	A	94	20.370	19.030	65.354	1.00	11.28
1405	NH1	ARG	A	94	19.745	19.754	64.435	1.00	11.42
1408	NH2	ARG	A	94	20.381	17.712	65.236	1.00	11.38
1411	C	ARG	A	94	25.356	17.977	65.286	1.00	9.74
1412	O	ARG	A	94	25.508	16.809	65.625	1.00	9.71
1413	N	LEU	A	95	25.051	18.339	64.041	1.00	9.85
1415	CA	LEU	A	95	24.798	17.355	62.989	1.00	10.10
1417	CB	LEU	A	95	24.336	18.042	61.699	1.00	9.96
1420	CG	LEU	A	95	22.972	18.735	61.732	1.00	9.83
1422	CD1	LEU	A	95	22.776	19.544	60.465	1.00	10.47
1426	CD2	LEU	A	95	21.847	17.734	61.901	1.00	10.58
1430	C	LEU	A	95	26.014	16.471	62.698	1.00	10.44
1431	O	LEU	A	95	25.860	15.295	62.374	1.00	10.47
1432	N	MSE	A	96	27.214	17.033	62.821	1.00	10.89
1434	CA	MSE	A	96	28.446	16.284	62.562	1.00	11.53
1436	CB	MSE	A	96	29.551	17.227	62.073	1.00	11.58
1439	CG	MSE	A	96	29.253	17.880	60.735	1.00	12.76
1442	SE	MSE	A	96	29.080	16.592	59.285	1.00	15.36
1443	CE	MSE	A	96	27.133	16.359	59.265	1.00	14.46
1447	C	MSE	A	96	28.945	15.499	63.782	1.00	11.55
1448	O	MSE	A	96	29.945	14.798	63.688	1.00	12.05
1449	N	GLY	A	97	28.265	15.627	64.920	1.00	11.70
1451	CA	GLY	A	97	28.626	14.905	66.131	1.00	11.68
1454	C	GLY	A	97	30.011	15.259	66.649	1.00	11.66
1455	O	GLY	A	97	30.722	14.407	67.191	1.00	11.30
1456	N	ILE	A	98	30.403	16.517	66.465	1.00	11.46
1458	CA	ILE	A	98	31.697	16.998	66.935	1.00	11.56
1460	CB	ILE	A	98	32.044	18.357	66.261	1.00	11.67
1462	CG1	ILE	A	98	32.386	18.121	64.783	1.00	12.15
1465	CD1	ILE	A	98	32.076	19.290	63.891	1.00	13.07
1469	CG2	ILE	A	98	33.213	19.060	66.957	1.00	11.73
1473	C	ILE	A	98	31.667	17.092	68.458	1.00	11.39
1474	O	ILE	A	98	30.633	17.401	69.047	1.00	11.30

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1475	N	GLN	A	99	32.800	16.795	69.088	1.00	11.46
1477	CA	GLN	A	99	32.905	16.809	70.547	1.00	11.54
1479	CB	GLN	A	99	34.324	16.428	71.007	1.00	11.48
1482	CG	GLN	A	99	35.434	17.381	70.554	1.00	11.36
1485	CD	GLN	A	99	35.666	18.553	71.498	1.00	11.13
1486	OE1	GLN	A	99	35.422	18.453	72.704	1.00	10.05
1487	NE2	GLN	A	99	36.141	19.668	70.948	1.00	10.34
1490	C	GLN	A	99	32.502	18.179	71.083	1.00	11.70
1491	O	GLN	A	99	32.718	19.201	70.412	1.00	11.69
1492	N	PRO	A	100	31.917	18.204	72.279	1.00	11.75
1493	CA	PRO	A	100	31.247	19.408	72.786	1.00	11.77
1495	CB	PRO	A	100	30.564	18.919	74.071	1.00	11.87
1498	CG	PRO	A	100	31.324	17.714	74.489	1.00	12.30
1501	CD	PRO	A	100	31.840	17.084	73.236	1.00	12.01
1504	C	PRO	A	100	32.154	20.606	73.088	1.00	11.66
1505	O	PRO	A	100	31.709	21.733	72.894	1.00	11.40
1506	N	PHE	A	101	33.374	20.379	73.568	1.00	11.39
1508	CA	PHE	A	101	34.247	21.482	73.971	1.00	11.08
1510	CB	PHE	A	101	35.238	21.024	75.039	1.00	11.24
1513	CG	PHE	A	101	34.570	20.585	76.308	1.00	12.06
1514	CD1	PHE	A	101	34.508	19.242	76.650	1.00	13.05
1516	CE1	PHE	A	101	33.875	18.835	77.817	1.00	13.37
1518	CZ	PHE	A	101	33.289	19.778	78.653	1.00	13.83
1520	CE2	PHE	A	101	33.339	21.118	78.319	1.00	13.49
1522	CD2	PHE	A	101	33.976	21.517	77.148	1.00	12.73
1524	C	PHE	A	101	34.940	22.141	72.779	1.00	10.89
1525	O	PHE	A	101	36.146	21.994	72.559	1.00	10.48
1526	N	ALA	A	102	34.139	22.896	72.032	1.00	10.37
1528	CA	ALA	A	102	34.557	23.531	70.799	1.00	10.37
1530	CB	ALA	A	102	34.195	22.653	69.624	1.00	10.31
1534	C	ALA	A	102	33.849	24.873	70.678	1.00	10.19
1535	O	ALA	A	102	32.712	25.018	71.122	1.00	9.89
1536	N	ARG	A	103	34.521	25.855	70.088	1.00	10.20
1538	CA	ARG	A	103	33.868	27.112	69.765	1.00	10.13
1540	CB	ARG	A	103	34.794	28.306	70.010	1.00	10.35
1543	CG	ARG	A	103	35.971	28.450	69.079	1.00	10.90
1546	CD	ARG	A	103	36.654	29.799	69.203	1.00	12.28
1549	NE	ARG	A	103	37.413	29.913	70.453	1.00	12.82
1551	CZ	ARG	A	103	38.734	29.763	70.561	1.00	13.92
1552	NH1	ARG	A	103	39.489	29.462	69.509	1.00	13.66
1555	NH2	ARG	A	103	39.308	29.897	71.748	1.00	14.54
1558	C	ARG	A	103	33.368	27.056	68.326	1.00	9.80
1559	O	ARG	A	103	34.030	26.502	67.451	1.00	9.76
1560	N	SER	A	104	32.180	27.608	68.101	1.00	9.40
1562	CA	SER	A	104	31.554	27.602	66.787	1.00	9.14
1564	CB	SER	A	104	30.402	26.595	66.754	1.00	9.08
1567	OG	SER	A	104	30.836	25.305	67.148	1.00	9.35
1569	C	SER	A	104	31.033	28.989	66.455	1.00	8.93
1570	O	SER	A	104	30.402	29.638	67.291	1.00	9.02
1571	N	PHE	A	105	31.300	29.451	65.239	1.00	8.58
1573	CA	PHE	A	105	30.807	30.753	64.810	1.00	8.44
1575	CB	PHE	A	105	31.632	31.886	65.446	1.00	8.51
1578	CG	PHE	A	105	33.110	31.809	65.163	1.00	8.77

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1579	CD1	PHE	A	105	33.652	32.439	64.050	1.00	9.46
1581	CE1	PHE	A	105	35.016	32.376	63.793	1.00	9.83
1583	CZ	PHE	A	105	35.850	31.680	64.657	1.00	9.82
1585	CE2	PHE	A	105	35.323	31.061	65.774	1.00	9.29
1587	CD2	PHE	A	105	33.959	31.127	66.023	1.00	9.41
1589	C	PHE	A	105	30.737	30.899	63.289	1.00	8.37
1590	O	PHE	A	105	31.187	30.039	62.533	1.00	8.04
1591	N	GLU	A	106	30.125	31.995	62.868	1.00	8.24
1593	CA	GLU	A	106	29.899	32.317	61.474	1.00	8.07
1595	CB	GLU	A	106	28.412	32.627	61.281	1.00	8.20
1598	CG	GLU	A	106	27.932	32.754	59.846	1.00	8.35
1601	CD	GLU	A	106	26.426	32.965	59.761	1.00	8.72
1602	OE1	GLU	A	106	25.997	34.028	59.278	1.00	8.98
1603	OE2	GLU	A	106	25.666	32.070	60.185	1.00	8.37
1604	C	GLU	A	106	30.747	33.542	61.145	1.00	8.13
1605	O	GLU	A	106	30.863	34.447	61.970	1.00	8.04
1606	N	ILE	A	107	31.364	33.550	59.966	1.00	7.95
1608	CA	ILE	A	107	32.082	34.718	59.465	1.00	8.06
1610	CB	ILE	A	107	33.538	34.376	59.089	1.00	8.03
1612	CG1	ILE	A	107	34.322	33.932	60.324	1.00	7.95
1615	CD1	ILE	A	107	35.773	33.575	60.051	1.00	8.07
1619	CG2	ILE	A	107	34.206	35.585	58.431	1.00	8.63
1623	C	ILE	A	107	31.358	35.251	58.242	1.00	8.20
1624	O	ILE	A	107	30.989	34.487	57.351	1.00	7.98
1625	N	LYS	A	108	31.165	36.567	58.213	1.00	8.27
1627	CA	LYS	A	108	30.539	37.257	57.102	1.00	8.05
1629	CB	LYS	A	108	29.251	37.934	57.574	1.00	8.27
1632	CG	LYS	A	108	28.519	38.748	56.506	1.00	7.91
1635	CD	LYS	A	108	27.625	39.815	57.123	1.00	7.62
1638	CE	LYS	A	108	26.417	39.204	57.820	1.00	7.37
1641	NZ	LYS	A	108	25.663	40.213	58.627	1.00	6.60
1645	C	LYS	A	108	31.482	38.314	56.537	1.00	8.22
1646	O	LYS	A	108	31.869	39.247	57.238	1.00	8.27
1647	N	GLU	A	109	31.863	38.135	55.274	1.00	7.96
1649	CA	GLU	A	109	32.377	39.210	54.436	1.00	8.10
1651	CB	GLU	A	109	33.819	39.604	54.810	1.00	8.20
1654	CG	GLU	A	109	34.553	40.569	53.870	1.00	8.27
1657	CD	GLU	A	109	33.658	41.419	52.973	1.00	8.80
1658	OE1	GLU	A	109	33.943	41.501	51.760	1.00	8.15
1659	OE2	GLU	A	109	32.687	42.021	53.466	1.00	7.88
1660	C	GLU	A	109	32.286	38.719	53.002	1.00	8.25
1661	O	GLU	A	109	33.284	38.315	52.412	1.00	8.36
1662	N	ALA	A	110	31.062	38.699	52.476	1.00	8.30
1664	CA	ALA	A	110	30.818	38.409	51.071	1.00	8.53
1666	CB	ALA	A	110	31.352	39.556	50.199	1.00	8.42
1670	C	ALA	A	110	31.444	37.051	50.715	1.00	8.69
1671	O	ALA	A	110	31.274	36.092	51.474	1.00	8.51
1672	N	CYS	A	111	32.172	36.962	49.600	1.00	8.92
1674	CA	CYS	A	111	32.778	35.694	49.172	1.00	9.35
1676	CB	CYS	A	111	32.860	35.642	47.650	1.00	9.57
1679	SG	CYS	A	111	31.241	35.528	46.894	1.00	12.01
1680	C	CYS	A	111	34.166	35.445	49.767	1.00	8.90
1681	O	CYS	A	111	34.855	34.504	49.368	1.00	8.75

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1682	N	TYR	A	112	34.562	36.289	50.715	1.00	8.51
1684	CA	TYR	A	112	35.842	36.171	51.398	1.00	8.49
1686	CB	TYR	A	112	36.433	37.572	51.639	1.00	8.45
1689	CG	TYR	A	112	37.714	37.558	52.438	1.00	8.23
1690	CD1	TYR	A	112	37.718	37.902	53.789	1.00	7.94
1692	CE1	TYR	A	112	38.879	37.862	54.531	1.00	7.59
1694	CZ	TYR	A	112	40.056	37.470	53.932	1.00	7.85
1695	OH	TYR	A	112	41.207	37.433	54.670	1.00	9.07
1697	CE2	TYR	A	112	40.083	37.122	52.594	1.00	7.85
1699	CD2	TYR	A	112	38.911	37.162	51.857	1.00	8.16
1701	C	TYR	A	112	35.732	35.399	52.727	1.00	8.56
1702	O	TYR	A	112	36.745	34.965	53.274	1.00	8.45
1703	N	GLY	A	113	34.510	35.212	53.225	1.00	8.46
1705	CA	GLY	A	113	34.287	34.679	54.563	1.00	8.51
1708	C	GLY	A	113	34.959	33.366	54.926	1.00	8.48
1709	O	GLY	A	113	35.472	33.223	56.039	1.00	8.59
1710	N	ALA	A	114	34.936	32.397	54.016	1.00	8.53
1712	CA	ALA	A	114	35.578	31.104	54.269	1.00	8.54
1714	CB	ALA	A	114	35.145	30.077	53.250	1.00	8.62
1718	C	ALA	A	114	37.105	31.210	54.301	1.00	8.33
1719	O	ALA	A	114	37.750	30.510	55.068	1.00	8.29
1720	N	THR	A	115	37.667	32.078	53.466	1.00	8.17
1722	CA	THR	A	115	39.105	32.345	53.464	1.00	7.94
1724	CB	THR	A	115	39.471	33.350	52.353	1.00	7.92
1726	OG1	THR	A	115	39.187	32.770	51.073	1.00	7.06
1728	CG2	THR	A	115	40.977	33.625	52.325	1.00	7.44
1732	C	THR	A	115	39.573	32.871	54.813	1.00	8.12
1733	O	THR	A	115	40.575	32.405	55.340	1.00	7.77
1734	N	ALA	A	116	38.842	33.835	55.370	1.00	8.24
1736	CA	ALA	A	116	39.132	34.329	56.707	1.00	8.43
1738	CB	ALA	A	116	38.110	35.374	57.119	1.00	8.68
1742	C	ALA	A	116	39.136	33.164	57.701	1.00	8.51
1743	O	ALA	A	116	40.024	33.065	58.536	1.00	8.28
1744	N	GLY	A	117	38.154	32.272	57.587	1.00	8.58
1746	CA	GLY	A	117	38.083	31.091	58.430	1.00	9.08
1749	C	GLY	A	117	39.288	30.171	58.283	1.00	9.55
1750	O	GLY	A	117	39.802	29.669	59.274	1.00	9.65
1751	N	LEU	A	118	39.736	29.959	57.048	1.00	10.21
1753	CA	LEU	A	118	40.879	29.085	56.763	1.00	10.89
1755	CB	LEU	A	118	41.087	28.956	55.251	1.00	10.87
1758	CG	LEU	A	118	42.324	28.178	54.785	1.00	10.58
1760	CD1	LEU	A	118	42.271	26.743	55.281	1.00	10.27
1764	CD2	LEU	A	118	42.431	28.226	53.273	1.00	10.81
1768	C	LEU	A	118	42.166	29.589	57.411	1.00	11.53
1769	O	LEU	A	118	42.910	28.808	57.993	1.00	11.49
1770	N	GLN	A	119	42.408	30.895	57.317	1.00	12.46
1772	CA	GLN	A	119	43.637	31.504	57.827	1.00	13.02
1774	CB	GLN	A	119	43.802	32.942	57.314	1.00	13.45
1777	CG	GLN	A	119	43.618	33.145	55.806	1.00	14.55
1780	CD	GLN	A	119	44.550	32.315	54.948	1.00	16.06
1781	OE1	GLN	A	119	45.334	31.516	55.453	1.00	18.97
1782	NE2	GLN	A	119	44.473	32.513	53.641	1.00	18.15
1785	C	GLN	A	119	43.658	31.514	59.344	1.00	13.14

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1786	O	GLN	A	119	44.692	31.275	59.957	1.00	13.12
1787	N	LEU	A	120	42.507	31.792	59.945	1.00	13.35
1789	CA	LEU	A	120	42.375	31.796	61.396	1.00	13.65
1791	CB	LEU	A	120	41.050	32.418	61.805	1.00	14.11
1794	CG	LEU	A	120	40.744	33.831	61.304	1.00	15.84
1796	CD1	LEU	A	120	41.577	34.872	62.009	1.00	17.23
1800	CD2	LEU	A	120	39.253	34.089	61.477	1.00	17.37
1804	C	LEU	A	120	42.463	30.372	61.956	1.00	13.27
1805	O	LEU	A	120	42.996	30.160	63.045	1.00	12.95
1806	N	ALA	A	121	41.942	29.405	61.203	1.00	12.70
1808	CA	ALA	A	121	42.070	27.996	61.564	1.00	12.46
1810	CB	ALA	A	121	41.259	27.123	60.616	1.00	12.45
1814	C	ALA	A	121	43.539	27.586	61.532	1.00	12.30
1815	O	ALA	A	121	44.004	26.867	62.411	1.00	12.02
1816	N	LYS	A	122	44.259	28.066	60.520	1.00	12.24
1818	CA	LYS	A	122	45.688	27.811	60.369	1.00	12.39
1820	CB	LYS	A	122	46.212	28.498	59.097	1.00	12.82
1823	CG	LYS	A	122	47.722	28.482	58.890	1.00	14.09
1826	CD	LYS	A	122	48.135	29.357	57.696	1.00	16.44
1829	CE	LYS	A	122	48.020	30.862	58.011	1.00	18.11
1832	NZ	LYS	A	122	48.699	31.750	57.010	1.00	19.35
1836	C	LYS	A	122	46.444	28.298	61.604	1.00	12.07
1837	O	LYS	A	122	47.277	27.579	62.142	1.00	11.46
1838	N	ASN	A	123	46.132	29.511	62.057	1.00	11.91
1840	CA	ASN	A	123	46.801	30.100	63.213	1.00	12.03
1842	CB	ASN	A	123	46.379	31.558	63.407	1.00	12.06
1845	CG	ASN	A	123	46.852	32.477	62.289	1.00	13.18
1846	OD1	ASN	A	123	46.371	33.604	62.175	1.00	16.00
1847	ND2	ASN	A	123	47.796	32.013	61.470	1.00	12.33
1850	C	ASN	A	123	46.509	29.316	64.491	1.00	11.82
1851	O	ASN	A	123	47.395	29.121	65.317	1.00	11.85
1852	N	HIS	A	124	45.262	28.870	64.635	1.00	11.73
1854	CA	HIS	A	124	44.811	28.096	65.793	1.00	11.68
1856	CB	HIS	A	124	43.282	27.909	65.729	1.00	11.67
1859	CG	HIS	A	124	42.732	26.956	66.749	1.00	11.58
1860	ND1	HIS	A	124	42.570	27.292	68.076	1.00	12.35
1862	CE1	HIS	A	124	42.064	26.263	68.731	1.00	12.28
1864	NE2	HIS	A	124	41.891	25.271	67.877	1.00	12.09
1866	CD2	HIS	A	124	42.299	25.679	66.631	1.00	11.67
1868	C	HIS	A	124	45.540	26.744	65.884	1.00	11.74
1869	O	HIS	A	124	45.940	26.328	66.967	1.00	11.33
1870	N	VAL	A	125	45.730	26.078	64.748	1.00	11.98
1872	CA	VAL	A	125	46.416	24.786	64.725	1.00	12.32
1874	CB	VAL	A	125	46.173	24.014	63.407	1.00	12.42
1876	CG1	VAL	A	125	46.966	22.714	63.389	1.00	12.42
1880	CG2	VAL	A	125	44.686	23.708	63.224	1.00	12.06
1884	C	VAL	A	125	47.916	24.981	64.970	1.00	12.81
1885	O	VAL	A	125	48.550	24.156	65.621	1.00	12.71
1886	N	ALA	A	126	48.472	26.086	64.479	1.00	13.25
1888	CA	ALA	A	126	49.879	26.397	64.699	1.00	13.63
1890	CB	ALA	A	126	50.257	27.723	64.026	1.00	13.69
1894	C	ALA	A	126	50.181	26.457	66.188	1.00	13.97
1895	O	ALA	A	126	51.231	26.006	66.628	1.00	13.99

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1896	N	LEU	A	127	49.241	27.001	66.955	1.00	14.43
1898	CA	LEU	A	127	49.413	27.177	68.393	1.00	14.74
1900	CB	LEU	A	127	48.655	28.420	68.860	1.00	14.90
1903	CG	LEU	A	127	49.404	29.753	68.731	1.00	15.69
1905	CD1	LEU	A	127	50.073	29.920	67.391	1.00	16.52
1909	CD2	LEU	A	127	48.456	30.894	68.961	1.00	16.12
1913	C	LEU	A	127	48.966	25.951	69.193	1.00	14.73
1914	O	LEU	A	127	49.373	25.777	70.338	1.00	14.56
1915	N	HIS	A	128	48.127	25.114	68.583	1.00	14.52
1917	CA	HIS	A	128	47.609	23.898	69.208	1.00	14.43
1919	CB	HIS	A	128	46.153	24.103	69.661	1.00	14.55
1922	CG	HIS	A	128	45.942	25.329	70.490	1.00	15.35
1923	ND1	HIS	A	128	46.328	25.411	71.811	1.00	16.64
1925	CE1	HIS	A	128	46.030	26.609	72.281	1.00	16.80
1927	NE2	HIS	A	128	45.460	27.305	71.314	1.00	16.52
1929	CD2	HIS	A	128	45.398	26.530	70.182	1.00	16.04
1931	C	HIS	A	128	47.689	22.772	68.171	1.00	14.17
1932	O	HIS	A	128	46.677	22.409	67.580	1.00	13.81
1933	N	PRO	A	129	48.890	22.238	67.928	1.00	14.20
1934	CA	PRO	A	129	49.129	21.375	66.756	1.00	14.22
1936	CB	PRO	A	129	50.654	21.151	66.761	1.00	14.34
1939	CG	PRO	A	129	51.212	21.889	67.923	1.00	14.71
1942	CD	PRO	A	129	50.098	22.420	68.749	1.00	14.36
1945	C	PRO	A	129	48.387	20.034	66.716	1.00	14.07
1946	O	PRO	A	129	48.372	19.413	65.654	1.00	13.54
1947	N	ASP	A	130	47.802	19.591	67.826	1.00	14.13
1949	CA	ASP	A	130	47.031	18.345	67.843	1.00	14.53
1951	CB	ASP	A	130	47.235	17.606	69.170	1.00	14.97
1954	CG	ASP	A	130	48.542	16.852	69.212	1.00	17.16
1955	OD1	ASP	A	130	49.007	16.505	70.321	1.00	19.49
1956	OD2	ASP	A	130	49.178	16.564	68.173	1.00	20.73
1957	C	ASP	A	130	45.540	18.573	67.601	1.00	14.17
1958	O	ASP	A	130	44.783	17.616	67.450	1.00	14.02
1959	N	LYS	A	131	45.123	19.834	67.570	1.00	13.78
1961	CA	LYS	A	131	43.730	20.174	67.308	1.00	13.67
1963	CB	LYS	A	131	43.336	21.445	68.062	1.00	13.85
1966	CG	LYS	A	131	43.532	21.369	69.571	1.00	15.14
1969	CD	LYS	A	131	42.730	20.237	70.206	1.00	16.93
1972	CE	LYS	A	131	42.857	20.254	71.721	1.00	18.42
1975	NZ	LYS	A	131	42.059	19.155	72.349	1.00	20.05
1979	C	LYS	A	131	43.483	20.354	65.819	1.00	13.04
1980	O	LYS	A	131	44.406	20.611	65.047	1.00	13.33
1981	N	LYS	A	132	42.225	20.203	65.427	1.00	12.41
1983	CA	LYS	A	132	41.801	20.403	64.049	1.00	11.95
1985	CB	LYS	A	132	41.384	19.069	63.419	1.00	11.87
1988	CG	LYS	A	132	42.485	18.008	63.418	1.00	12.18
1991	CD	LYS	A	132	42.055	16.738	62.684	1.00	12.64
1994	CE	LYS	A	132	43.042	15.580	62.920	1.00	13.88
1997	NZ	LYS	A	132	42.723	14.399	62.054	1.00	14.60
2001	C	LYS	A	132	40.649	21.411	64.014	1.00	11.55
2002	O	LYS	A	132	40.044	21.724	65.041	1.00	11.06
2003	N	VAL	A	133	40.369	21.932	62.825	1.00	11.00
2005	CA	VAL	A	133	39.317	22.922	62.643	1.00	10.59

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2007	CB	VAL	A	133	39.903	24.339	62.483	1.00	10.69
2009	CG1	VAL	A	133	38.787	25.383	62.357	1.00	10.86
2013	CG2	VAL	A	133	40.825	24.674	63.650	1.00	10.72
2017	C	VAL	A	133	38.513	22.566	61.403	1.00	10.26
2018	O	VAL	A	133	39.086	22.259	60.361	1.00	9.85
2019	N	LEU	A	134	37.188	22.586	61.527	1.00	9.94
2021	CA	LEU	A	134	36.303	22.427	60.380	1.00	9.68
2023	CB	LEU	A	134	35.059	21.616	60.759	1.00	9.64
2026	CG	LEU	A	134	33.986	21.460	59.676	1.00	9.49
2028	CD1	LEU	A	134	34.510	20.649	58.499	1.00	9.95
2032	CD2	LEU	A	134	32.735	20.827	60.246	1.00	9.09
2036	C	LEU	A	134	35.910	23.811	59.884	1.00	9.54
2037	O	LEU	A	134	35.357	24.605	60.638	1.00	9.41
2038	N	VAL	A	135	36.232	24.097	58.625	1.00	9.38
2040	CA	VAL	A	135	35.868	25.349	57.974	1.00	9.26
2042	CB	VAL	A	135	37.110	26.128	57.506	1.00	9.28
2044	CG1	VAL	A	135	36.702	27.435	56.799	1.00	9.56
2048	CG2	VAL	A	135	38.032	26.420	58.683	1.00	9.40
2052	C	VAL	A	135	35.017	25.008	56.765	1.00	9.01
2053	O	VAL	A	135	35.452	24.261	55.906	1.00	9.07
2054	N	VAL	A	136	33.805	25.547	56.705	1.00	8.85
2056	CA	VAL	A	136	32.890	25.265	55.607	1.00	8.69
2058	CB	VAL	A	136	31.669	24.451	56.076	1.00	8.63
2060	CG1	VAL	A	136	30.798	24.056	54.883	1.00	8.60
2064	CG2	VAL	A	136	32.105	23.216	56.856	1.00	8.66
2068	C	VAL	A	136	32.391	26.552	54.969	1.00	8.66
2069	O	VAL	A	136	31.784	27.392	55.635	1.00	9.26
2070	N	ALA	A	137	32.669	26.706	53.679	1.00	8.40
2072	CA	ALA	A	137	32.022	27.712	52.852	1.00	8.10
2074	CB	ALA	A	137	32.859	27.975	51.616	1.00	8.23
2078	C	ALA	A	137	30.658	27.168	52.452	1.00	7.88
2079	O	ALA	A	137	30.564	26.045	51.974	1.00	7.70
2080	N	ALA	A	138	29.604	27.946	52.657	1.00	7.43
2082	CA	ALA	A	138	28.262	27.537	52.251	1.00	7.40
2084	CB	ALA	A	138	27.589	26.769	53.365	1.00	7.40
2088	C	ALA	A	138	27.432	28.760	51.859	1.00	7.37
2089	O	ALA	A	138	27.448	29.785	52.543	1.00	7.17
2090	N	ASP	A	139	26.707	28.649	50.756	1.00	7.60
2092	CA	ASP	A	139	26.025	29.804	50.177	1.00	7.67
2094	CB	ASP	A	139	27.048	30.772	49.559	1.00	7.67
2097	CG	ASP	A	139	27.526	31.841	50.526	1.00	7.79
2098	OD1	ASP	A	139	26.684	32.509	51.159	1.00	7.08
2099	OD2	ASP	A	139	28.739	32.089	50.713	1.00	7.82
2100	C	ASP	A	139	25.030	29.404	49.100	1.00	7.68
2101	O	ASP	A	139	25.143	28.342	48.480	1.00	7.56
2102	N	ILE	A	140	24.058	30.283	48.884	1.00	7.73
2104	CA	ILE	A	140	23.115	30.187	47.781	1.00	7.89
2106	CB	ILE	A	140	21.688	29.955	48.317	1.00	7.98
2108	CG1	ILE	A	140	21.574	28.567	48.953	1.00	7.66
2111	CD1	ILE	A	140	20.487	28.472	49.996	1.00	8.00
2115	CG2	ILE	A	140	20.648	30.111	47.202	1.00	7.70
2119	C	ILE	A	140	23.184	31.508	47.020	1.00	8.26
2120	O	ILE	A	140	22.756	32.544	47.532	1.00	8.00

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2121	N	ALA	A	141	23.742	31.465	45.811	1.00	8.66
2123	CA	ALA	A	141	23.851	32.641	44.950	1.00	9.05
2125	CB	ALA	A	141	25.141	32.582	44.149	1.00	8.98
2129	C	ALA	A	141	22.646	32.783	44.020	1.00	9.34
2130	O	ALA	A	141	22.586	32.152	42.962	1.00	9.52
2131	N	LYS	A	142	21.688	33.609	44.441	1.00	9.81
2133	CA	LYS	A	142	20.492	33.927	43.667	1.00	10.11
2135	CB	LYS	A	142	19.244	33.435	44.404	1.00	10.11
2138	CG	LYS	A	142	19.073	31.923	44.412	1.00	10.30
2141	CD	LYS	A	142	17.929	31.479	45.328	1.00	10.41
2144	CE	LYS	A	142	16.563	31.579	44.646	1.00	10.11
2147	NZ	LYS	A	142	15.512	30.779	45.356	1.00	9.92
2151	C	LYS	A	142	20.391	35.441	43.450	1.00	10.40
2152	O	LYS	A	142	20.428	36.213	44.415	1.00	10.68
2153	N	TYR	A	143	20.262	35.851	42.187	1.00	10.40
2155	CA	TYR	A	143	20.173	37.266	41.807	1.00	10.45
2157	CB	TYR	A	143	21.115	37.559	40.639	1.00	10.34
2160	CG	TYR	A	143	22.571	37.658	41.025	1.00	10.19
2161	CD1	TYR	A	143	23.410	36.554	40.943	1.00	10.20
2163	CE1	TYR	A	143	24.756	36.643	41.295	1.00	9.77
2165	CZ	TYR	A	143	25.271	37.851	41.721	1.00	10.11
2166	OH	TYR	A	143	26.597	37.946	42.062	1.00	9.94
2168	CE2	TYR	A	143	24.458	38.968	41.807	1.00	10.39
2170	CD2	TYR	A	143	23.116	38.867	41.459	1.00	10.62
2172	C	TYR	A	143	18.762	37.699	41.415	1.00	10.67
2173	O	TYR	A	143	18.375	38.851	41.638	1.00	10.26
2174	N	GLY	A	144	18.019	36.784	40.797	1.00	10.86
2176	CA	GLY	A	144	16.657	37.040	40.370	1.00	11.24
2179	C	GLY	A	144	16.453	36.603	38.931	1.00	11.57
2180	O	GLY	A	144	17.376	36.662	38.111	1.00	11.55
2181	N	LEU	A	145	15.238	36.165	38.627	1.00	11.92
2183	CA	LEU	A	145	14.871	35.794	37.270	1.00	12.48
2185	CB	LEU	A	145	13.484	35.149	37.248	1.00	12.67
2188	CG	LEU	A	145	13.302	33.876	38.082	1.00	13.43
2190	CD1	LEU	A	145	11.839	33.450	38.066	1.00	14.02
2194	CD2	LEU	A	145	14.191	32.747	37.588	1.00	14.37
2198	C	LEU	A	145	14.895	37.041	36.383	1.00	12.71
2199	O	LEU	A	145	14.393	38.094	36.774	1.00	12.20
2200	N	ASN	A	146	15.483	36.899	35.195	1.00	13.10
2202	CA	ASN	A	146	15.672	37.994	34.243	1.00	13.64
2204	CB	ASN	A	146	14.313	38.566	33.808	1.00	14.03
2207	CG	ASN	A	146	13.440	37.521	33.153	1.00	14.84
2208	OD1	ASN	A	146	13.721	37.083	32.042	1.00	16.89
2209	ND2	ASN	A	146	12.391	37.095	33.847	1.00	16.12
2212	C	ASN	A	146	16.605	39.108	34.722	1.00	13.76
2213	O	ASN	A	146	16.589	40.211	34.173	1.00	14.21
2214	N	SER	A	147	17.434	38.815	35.721	1.00	13.67
2216	CA	SER	A	147	18.389	39.787	36.242	1.00	13.63
2218	CB	SER	A	147	18.606	39.582	37.745	1.00	13.62
2221	OG	SER	A	147	19.282	38.366	38.013	1.00	13.22
2223	C	SER	A	147	19.712	39.673	35.488	1.00	13.63
2224	O	SER	A	147	19.980	38.662	34.832	1.00	13.87
2225	N	GLY	A	148	20.533	40.716	35.575	1.00	13.52

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2227	CA	GLY	A	148	21.849	40.713	34.958	1.00	13.38
2230	C	GLY	A	148	22.749	39.629	35.530	1.00	13.14
2231	O	GLY	A	148	23.518	38.999	34.801	1.00	13.57
2232	N	GLY	A	149	22.636	39.397	36.836	1.00	12.78
2234	CA	GLY	A	149	23.474	38.432	37.528	1.00	12.37
2237	C	GLY	A	149	23.030	36.981	37.414	1.00	12.09
2238	O	GLY	A	149	23.775	36.088	37.812	1.00	11.90
2239	N	GLU	A	150	21.839	36.744	36.862	1.00	11.62
2241	CA	GLU	A	150	21.231	35.406	36.850	1.00	11.65
2243	CB	GLU	A	150	19.874	35.425	36.130	1.00	11.55
2246	CG	GLU	A	150	19.063	34.146	36.312	1.00	11.84
2249	CD	GLU	A	150	17.831	34.090	35.431	1.00	12.30
2250	OE1	GLU	A	150	17.666	34.968	34.556	1.00	11.88
2251	OE2	GLU	A	150	17.023	33.160	35.618	1.00	12.75
2252	C	GLU	A	150	22.088	34.280	36.259	1.00	11.47
2253	O	GLU	A	150	22.097	33.178	36.811	1.00	11.26
2254	N	PRO	A	151	22.763	34.515	35.133	1.00	11.33
2255	CA	PRO	A	151	23.605	33.472	34.526	1.00	11.30
2257	CB	PRO	A	151	24.141	34.144	33.255	1.00	11.34
2260	CG	PRO	A	151	23.224	35.266	32.996	1.00	11.39
2263	CD	PRO	A	151	22.765	35.748	34.325	1.00	11.43
2266	C	PRO	A	151	24.770	32.999	35.403	1.00	10.92
2267	O	PRO	A	151	25.282	31.904	35.174	1.00	11.23
2268	N	THR	A	152	25.178	33.807	36.378	1.00	10.60
2270	CA	THR	A	152	26.276	33.456	37.282	1.00	10.18
2272	CB	THR	A	152	27.086	34.717	37.661	1.00	10.21
2274	OG1	THR	A	152	26.318	35.566	38.529	1.00	10.12
2276	CG2	THR	A	152	27.381	35.576	36.426	1.00	9.78
2280	C	THR	A	152	25.827	32.742	38.557	1.00	10.14
2281	O	THR	A	152	26.650	32.469	39.432	1.00	9.99
2282	N	GLN	A	153	24.538	32.430	38.657	1.00	9.86
2284	CA	GLN	A	153	23.969	31.833	39.864	1.00	9.69
2286	CB	GLN	A	153	22.441	31.772	39.758	1.00	9.87
2289	CG	GLN	A	153	21.752	33.121	39.943	1.00	9.53
2292	CD	GLN	A	153	20.264	33.095	39.626	1.00	9.61
2293	OE1	GLN	A	153	19.578	34.096	39.803	1.00	10.05
2294	NE2	GLN	A	153	19.764	31.956	39.163	1.00	10.14
2297	C	GLN	A	153	24.514	30.432	40.143	1.00	9.50
2298	O	GLN	A	153	25.005	29.749	39.248	1.00	9.22
2299	N	GLY	A	154	24.412	30.025	41.403	1.00	9.32
2301	CA	GLY	A	154	24.827	28.701	41.841	1.00	9.29
2304	C	GLY	A	154	24.465	28.458	43.298	1.00	9.23
2305	O	GLY	A	154	23.792	29.279	43.917	1.00	9.03
2306	N	ALA	A	155	24.908	27.329	43.844	1.00	9.22
2308	CA	ALA	A	155	24.603	26.970	45.236	1.00	9.24
2310	CB	ALA	A	155	23.108	26.732	45.419	1.00	9.26
2314	C	ALA	A	155	25.373	25.733	45.674	1.00	9.36
2315	O	ALA	A	155	25.624	24.833	44.870	1.00	9.41
2316	N	GLY	A	156	25.723	25.683	46.958	1.00	9.14
2318	CA	GLY	A	156	26.509	24.587	47.486	1.00	9.00
2321	C	GLY	A	156	27.404	24.960	48.649	1.00	8.94
2322	O	GLY	A	156	27.261	26.021	49.257	1.00	8.71
2323	N	ALA	A	157	28.334	24.061	48.950	1.00	8.95

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2325	CA	ALA	A	157	29.261	24.218	50.058	1.00	8.73
2327	CB	ALA	A	157	28.649	23.656	51.327	1.00	9.01
2331	C	ALA	A	157	30.583	23.515	49.760	1.00	9.11
2332	O	ALA	A	157	30.639	22.580	48.959	1.00	8.66
2333	N	VAL	A	158	31.649	23.999	50.383	1.00	9.22
2335	CA	VAL	A	158	32.941	23.330	50.358	1.00	9.60
2337	CB	VAL	A	158	33.978	24.108	49.521	1.00	9.65
2339	CG1	VAL	A	158	35.328	23.395	49.531	1.00	10.09
2343	CG2	VAL	A	158	33.485	24.300	48.088	1.00	10.12
2347	C	VAL	A	158	33.429	23.233	51.796	1.00	9.65
2348	O	VAL	A	158	33.571	24.252	52.471	1.00	9.33
2349	N	ALA	A	159	33.667	22.006	52.253	1.00	9.67
2351	CA	ALA	A	159	34.161	21.744	53.598	1.00	9.72
2353	CB	ALA	A	159	33.394	20.591	54.223	1.00	9.65
2357	C	ALA	A	159	35.644	21.421	53.558	1.00	9.92
2358	O	ALA	A	159	36.111	20.731	52.652	1.00	9.97
2359	N	MSE	A	160	36.366	21.912	54.561	1.00	9.85
2361	CA	MSE	A	160	37.807	21.740	54.676	1.00	10.25
2363	CB	MSE	A	160	38.525	23.048	54.332	1.00	10.33
2366	CG	MSE	A	160	38.599	23.355	52.855	1.00	11.81
2369	SE	MSE	A	160	39.220	25.196	52.551	1.00	16.07
2370	CE	MSE	A	160	37.567	26.133	52.909	1.00	15.45
2374	C	MSE	A	160	38.172	21.352	56.101	1.00	9.83
2375	O	MSE	A	160	37.702	21.970	57.052	1.00	10.11
2376	N	LEU	A	161	39.009	20.332	56.248	1.00	9.54
2378	CA	LEU	A	161	39.587	19.997	57.541	1.00	9.30
2380	CB	LEU	A	161	39.620	18.486	57.765	1.00	9.38
2383	CG	LEU	A	161	40.029	18.052	59.176	1.00	9.40
2385	CD1	LEU	A	161	38.957	18.433	60.216	1.00	9.53
2389	CD2	LEU	A	161	40.317	16.565	59.210	1.00	9.63
2393	C	LEU	A	161	40.993	20.577	57.579	1.00	9.21
2394	O	LEU	A	161	41.837	20.227	56.758	1.00	8.91
2395	N	VAL	A	162	41.220	21.492	58.514	1.00	9.26
2397	CA	VAL	A	162	42.504	22.153	58.677	1.00	9.34
2399	CB	VAL	A	162	42.314	23.657	58.975	1.00	9.39
2401	CG1	VAL	A	162	43.645	24.353	59.162	1.00	9.25
2405	CG2	VAL	A	162	41.514	24.328	57.849	1.00	9.48
2409	C	VAL	A	162	43.233	21.457	59.823	1.00	9.57
2410	O	VAL	A	162	42.665	21.254	60.895	1.00	9.48
2411	N	ALA	A	163	44.488	21.087	59.594	1.00	9.96
2413	CA	ALA	A	163	45.246	20.303	60.567	1.00	10.16
2415	CB	ALA	A	163	44.794	18.851	60.517	1.00	10.29
2419	C	ALA	A	163	46.748	20.378	60.338	1.00	10.35
2420	O	ALA	A	163	47.214	20.822	59.287	1.00	10.41
2421	N	SER	A	164	47.496	19.943	61.347	1.00	10.54
2423	CA	SER	A	164	48.933	19.719	61.228	1.00	10.62
2425	CB	ASER	A	164	49.551	19.436	62.602	0.65	10.46
2428	OG	ASER	A	164	49.589	20.613	63.387	0.65	10.35
2430	C	SER	A	164	49.213	18.548	60.289	1.00	10.78
2431	O	SER	A	164	48.393	17.640	60.156	1.00	10.59
2432	N	GLU	A	165	50.382	18.576	59.655	1.00	11.10
2434	CA	GLU	A	165	50.777	17.573	58.667	1.00	11.46
2436	CB	GLU	A	165	51.269	16.304	59.380	1.00	12.06

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2439	CG	GLU	A	165	52.429	16.547	60.341	1.00	13.61
2442	CD	GLU	A	165	53.615	17.200	59.665	1.00	15.76
2443	OE1	GLU	A	165	54.131	16.613	58.687	1.00	18.61
2444	OE2	GLU	A	165	54.023	18.305	60.095	1.00	17.31
2445	C	GLU	A	165	49.651	17.248	57.676	1.00	11.24
2446	O	GLU	A	165	49.270	16.087	57.510	1.00	10.92
2447	N	PRO	A	166	49.127	18.271	56.999	1.00	10.93
2448	CA	PRO	A	166	47.983	18.079	56.102	1.00	10.91
2450	CB	PRO	A	166	47.660	19.504	55.646	1.00	10.85
2453	CG	PRO	A	166	48.971	20.202	55.723	1.00	10.89
2456	CD	PRO	A	166	49.605	19.664	56.974	1.00	10.93
2459	C	PRO	A	166	48.367	17.209	54.913	1.00	10.94
2460	O	PRO	A	166	49.510	17.253	54.466	1.00	10.53
2461	N	ARG	A	167	47.419	16.428	54.411	1.00	11.26
2463	CA	ARG	A	167	47.697	15.496	53.330	1.00	11.78
2465	CB	ARG	A	167	46.844	14.233	53.491	1.00	12.00
2468	CG	ARG	A	167	47.414	13.295	54.549	1.00	13.51
2471	CD	ARG	A	167	46.535	12.105	54.859	1.00	15.69
2474	NE	ARG	A	167	45.383	12.474	55.681	1.00	16.29
2476	CZ	ARG	A	167	44.367	11.660	55.957	1.00	17.66
2477	NH1	ARG	A	167	44.346	10.415	55.499	1.00	18.68
2480	NH2	ARG	A	167	43.362	12.092	56.704	1.00	18.00
2483	C	ARG	A	167	47.540	16.100	51.928	1.00	11.71
2484	O	ARG	A	167	47.971	15.487	50.960	1.00	11.52
2485	N	ILE	A	168	46.962	17.297	51.814	1.00	11.78
2487	CA	ILE	A	168	46.747	17.908	50.495	1.00	11.82
2489	CB	ILE	A	168	45.243	18.166	50.239	1.00	11.94
2491	CG1	ILE	A	168	44.481	16.833	50.206	1.00	12.52
2494	CD1	ILE	A	168	42.981	16.965	50.345	1.00	12.95
2498	CG2	ILE	A	168	45.040	18.912	48.913	1.00	11.64
2502	C	ILE	A	168	47.575	19.175	50.261	1.00	11.73
2503	O	ILE	A	168	48.413	19.202	49.361	1.00	11.69
2504	N	LEU	A	169	47.335	20.217	51.052	1.00	11.78
2506	CA	LEU	A	169	47.941	21.523	50.815	1.00	11.87
2508	CB	LEU	A	169	46.906	22.464	50.192	1.00	11.71
2511	CG	LEU	A	169	47.416	23.762	49.559	1.00	11.64
2513	CD1	LEU	A	169	48.135	23.480	48.252	1.00	11.68
2517	CD2	LEU	A	169	46.264	24.741	49.332	1.00	11.66
2521	C	LEU	A	169	48.503	22.137	52.099	1.00	12.17
2522	O	LEU	A	169	47.756	22.442	53.021	1.00	12.38
2523	N	ALA	A	170	49.822	22.298	52.149	1.00	12.45
2525	CA	ALA	A	170	50.502	22.980	53.251	1.00	12.68
2527	CB	ALA	A	170	51.923	22.447	53.391	1.00	12.67
2531	C	ALA	A	170	50.529	24.494	52.994	1.00	13.02
2532	O	ALA	A	170	51.084	24.941	51.994	1.00	13.05
2533	N	LEU	A	171	49.933	25.273	53.892	1.00	13.30
2535	CA	LEU	A	171	49.847	26.729	53.735	1.00	13.74
2537	CB	LEU	A	171	48.643	27.267	54.514	1.00	13.75
2540	CG	LEU	A	171	47.285	26.676	54.126	1.00	13.45
2542	CD1	LEU	A	171	46.208	27.199	55.055	1.00	13.54
2546	CD2	LEU	A	171	46.945	26.985	52.674	1.00	13.44
2550	C	LEU	A	171	51.117	27.485	54.161	1.00	14.39
2551	O	LEU	A	171	51.699	27.212	55.215	1.00	14.08

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2552	N	LYS	A	172	51.522	28.447	53.333	1.00	15.09
2554	CA	LYS	A	172	52.697	29.283	53.588	1.00	16.02
2556	CB	LYS	A	172	53.357	29.681	52.267	1.00	16.24
2559	CG	LYS	A	172	53.726	28.519	51.360	1.00	17.61
2562	CD	LYS	A	172	54.865	27.687	51.925	1.00	19.43
2565	CE	LYS	A	172	55.694	27.054	50.808	1.00	20.67
2568	NZ	LYS	A	172	56.483	25.886	51.299	1.00	20.97
2572	C	LYS	A	172	52.308	30.548	54.362	1.00	16.28
2573	O	LYS	A	172	51.127	30.810	54.583	1.00	16.26
2574	N	GLU	A	173	53.306	31.337	54.754	1.00	16.75
2576	CA	GLU	A	173	53.078	32.555	55.534	1.00	17.09
2578	CB	GLU	A	173	53.994	32.566	56.771	1.00	17.42
2581	CG	GLU	A	173	53.625	31.526	57.821	1.00	18.72
2584	CD	GLU	A	173	52.260	31.774	58.436	1.00	20.65
2585	OE1	GLU	A	173	51.387	30.887	58.336	1.00	22.61
2586	OE2	GLU	A	173	52.056	32.861	59.013	1.00	22.84
2587	C	GLU	A	173	53.292	33.823	54.702	1.00	16.94
2588	O	GLU	A	173	53.699	34.855	55.234	1.00	17.36
2589	N	ASP	A	174	52.982	33.754	53.410	1.00	16.40
2591	CA	ASP	A	174	53.199	34.879	52.491	1.00	16.18
2593	CB	ASP	A	174	53.844	34.380	51.189	1.00	16.21
2596	CG	ASP	A	174	52.908	33.516	50.350	1.00	16.32
2597	OD1	ASP	A	174	51.965	32.913	50.909	1.00	16.12
2598	OD2	ASP	A	174	53.050	33.378	49.115	1.00	16.66
2599	C	ASP	A	174	51.917	35.675	52.189	1.00	15.69
2600	O	ASP	A	174	51.791	36.277	51.123	1.00	15.42
2601	N	ASN	A	175	51.002	35.714	53.155	1.00	15.39
2603	CA	ASN	A	175	49.680	36.311	52.969	1.00	15.40
2605	CB	ASN	A	175	48.796	36.082	54.208	1.00	15.65
2608	CG	ASN	A	175	48.653	34.609	54.575	1.00	16.38
2609	OD1	ASN	A	175	49.614	33.970	55.013	1.00	17.33
2610	ND2	ASN	A	175	47.449	34.069	54.410	1.00	16.77
2613	C	ASN	A	175	49.755	37.817	52.702	1.00	14.93
2614	O	ASN	A	175	50.455	38.539	53.411	1.00	14.79
2615	N	VAL	A	176	49.041	38.276	51.676	1.00	14.38
2617	CA	VAL	A	176	48.820	39.704	51.444	1.00	13.96
2619	CB	VAL	A	176	49.479	40.189	50.142	1.00	13.89
2621	CG1	VAL	A	176	49.216	41.686	49.933	1.00	13.89
2625	CG2	VAL	A	176	50.975	39.897	50.155	1.00	13.82
2629	C	VAL	A	176	47.319	39.977	51.361	1.00	13.73
2630	O	VAL	A	176	46.641	39.458	50.484	1.00	13.61
2631	N	MSE	A	177	46.821	40.810	52.265	1.00	13.44
2633	CA	MSE	A	177	45.400	41.126	52.355	1.00	13.57
2635	CB	MSE	A	177	44.917	40.898	53.783	1.00	14.27
2638	CG	MSE	A	177	45.227	39.509	54.276	1.00	17.42
2641	SE	MSE	A	177	46.866	39.452	55.287	1.00	25.32
2642	CE	MSE	A	177	46.098	40.044	56.963	1.00	20.95
2646	C	MSE	A	177	45.135	42.562	51.950	1.00	12.52
2647	O	MSE	A	177	46.062	43.365	51.856	1.00	12.00
2648	N	LEU	A	178	43.861	42.874	51.729	1.00	11.51
2650	CA	LEU	A	178	43.431	44.195	51.274	1.00	10.81
2652	CB	LEU	A	178	43.549	44.293	49.754	1.00	10.73
2655	CG	LEU	A	178	43.062	45.590	49.104	1.00	10.48

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2657	CD1	LEU	A	178	43.974	46.756	49.475	1.00	10.91
2661	CD2	LEU	A	178	42.976	45.428	47.595	1.00	10.18
2665	C	LEU	A	178	41.988	44.476	51.686	1.00	10.49
2666	O	LEU	A	178	41.126	43.613	51.551	1.00	10.69
2667	N	THR	A	179	41.738	45.681	52.189	1.00	9.92
2669	CA	THR	A	179	40.386	46.157	52.463	1.00	9.76
2671	CB	THR	A	179	40.099	46.227	53.983	1.00	9.58
2673	OG1	THR	A	179	40.141	44.918	54.561	1.00	9.01
2675	CG2	THR	A	179	38.666	46.691	54.241	1.00	9.54
2679	C	THR	A	179	40.204	47.542	51.850	1.00	9.95
2680	O	THR	A	179	41.029	48.431	52.053	1.00	9.68
2681	N	GLN	A	180	39.125	47.698	51.093	1.00	10.38
2683	CA	GLN	A	180	38.723	48.972	50.500	1.00	10.89
2685	CB	GLN	A	180	39.103	49.022	49.019	1.00	11.29
2688	CG	GLN	A	180	40.588	49.011	48.731	1.00	13.32
2691	CD	GLN	A	180	40.878	48.810	47.255	1.00	16.17
2692	OE1	GLN	A	180	40.339	47.894	46.632	1.00	19.30
2693	NE2	GLN	A	180	41.726	49.659	46.695	1.00	18.52
2696	C	GLN	A	180	37.215	49.062	50.594	1.00	10.59
2697	O	GLN	A	180	36.522	48.139	50.184	1.00	10.83
2698	N	ASP	A	181	36.695	50.166	51.110	1.00	10.21
2700	CA	ASP	A	181	35.250	50.339	51.224	1.00	10.01
2702	CB	ASP	A	181	34.940	51.394	52.289	1.00	10.05
2705	CG	ASP	A	181	33.456	51.509	52.606	1.00	10.32
2706	OD1	ASP	A	181	32.615	50.849	51.952	1.00	9.35
2707	OD2	ASP	A	181	33.039	52.263	53.509	1.00	10.08
2708	C	ASP	A	181	34.657	50.727	49.862	1.00	9.83
2709	O	ASP	A	181	34.656	51.899	49.488	1.00	9.57
2710	N	ILE	A	182	34.177	49.723	49.124	1.00	9.65
2712	CA	ILE	A	182	33.582	49.906	47.797	1.00	9.51
2714	CB	ILE	A	182	34.546	49.379	46.698	1.00	9.85
2716	CG1	ILE	A	182	35.866	50.163	46.698	1.00	10.58
2719	CD1	ILE	A	182	37.031	49.410	46.068	1.00	11.59
2723	CG2	ILE	A	182	33.889	49.454	45.311	1.00	9.86
2727	C	ILE	A	182	32.255	49.145	47.716	1.00	9.36
2728	O	ILE	A	182	32.189	47.967	48.072	1.00	9.29
2729	N	TYR	A	183	31.206	49.810	47.235	1.00	8.98
2731	CA	TYR	A	183	29.889	49.186	47.098	1.00	8.58
2733	CB	TYR	A	183	28.780	50.159	47.512	1.00	8.77
2736	CG	TYR	A	183	28.601	50.230	49.009	1.00	8.16
2737	CD1	TYR	A	183	27.776	49.325	49.668	1.00	8.38
2739	CE1	TYR	A	183	27.609	49.372	51.036	1.00	8.36
2741	CZ	TYR	A	183	28.280	50.324	51.777	1.00	8.58
2742	OH	TYR	A	183	28.104	50.361	53.139	1.00	8.59
2744	CE2	TYR	A	183	29.114	51.236	51.153	1.00	8.23
2746	CD2	TYR	A	183	29.276	51.181	49.771	1.00	8.47
2748	C	TYR	A	183	29.678	48.658	45.675	1.00	8.55
2749	O	TYR	A	183	28.853	49.163	44.913	1.00	8.15
2750	N	ASP	A	184	30.456	47.635	45.335	1.00	8.32
2752	CA	ASP	A	184	30.312	46.932	44.066	1.00	8.18
2754	CB	ASP	A	184	31.622	46.248	43.661	1.00	8.22
2757	CG	ASP	A	184	32.101	45.209	44.673	1.00	8.18
2758	OD1	ASP	A	184	32.535	44.115	44.246	1.00	8.68

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2759	OD2	ASP	A	184	32.088	45.394	45.911	1.00	7.47
2760	C	ASP	A	184	29.175	45.916	44.140	1.00	8.24
2761	O	ASP	A	184	28.450	45.707	43.168	1.00	7.84
2762	N	PHE	A	185	29.037	45.295	45.306	1.00	8.04
2764	CA	PHE	A	185	28.040	44.267	45.542	1.00	7.89
2766	CB	PHE	A	185	28.508	42.943	44.915	1.00	7.75
2769	CG	PHE	A	185	27.760	41.702	45.371	1.00	7.63
2770	CD1	PHE	A	185	27.087	40.911	44.441	1.00	7.45
2772	CE1	PHE	A	185	26.432	39.750	44.830	1.00	7.90
2774	CZ	PHE	A	185	26.444	39.357	46.156	1.00	7.91
2776	CE2	PHE	A	185	27.116	40.120	47.092	1.00	7.43
2778	CD2	PHE	A	185	27.782	41.281	46.699	1.00	7.90
2780	C	PHE	A	185	27.843	44.191	47.054	1.00	7.70
2781	O	PHE	A	185	28.804	44.200	47.827	1.00	7.20
2782	N	TRP	A	186	26.579	44.158	47.454	1.00	7.77
2784	CA	TRP	A	186	26.188	44.121	48.854	1.00	7.97
2786	CB	TRP	A	186	26.418	45.494	49.511	1.00	8.09
2789	CG	TRP	A	186	25.474	46.599	49.098	1.00	8.54
2790	CD1	TRP	A	186	24.474	47.130	49.855	1.00	8.87
2792	NE1	TRP	A	186	23.829	48.126	49.164	1.00	9.00
2794	CE2	TRP	A	186	24.421	48.279	47.939	1.00	8.41
2795	CD2	TRP	A	186	25.464	47.332	47.857	1.00	8.64
2796	CE3	TRP	A	186	26.232	47.286	46.683	1.00	8.84
2798	CZ3	TRP	A	186	25.930	48.162	45.647	1.00	8.24
2800	CH2	TRP	A	186	24.882	49.087	45.763	1.00	8.87
2802	CZ2	TRP	A	186	24.117	49.159	46.897	1.00	8.83
2804	C	TRP	A	186	24.726	43.660	48.944	1.00	8.31
2805	O	TRP	A	186	24.062	43.491	47.924	1.00	7.89
2806	N	ARG	A	187	24.240	43.411	50.153	1.00	8.44
2808	CA	ARG	A	187	22.861	42.965	50.333	1.00	8.63
2810	CB	ARG	A	187	22.767	41.437	50.300	1.00	8.69
2813	CG	ARG	A	187	21.335	40.924	50.245	1.00	8.68
2816	CD	ARG	A	187	21.186	39.557	49.596	1.00	9.08
2819	NE	ARG	A	187	21.676	38.478	50.454	1.00	8.27
2821	CZ	ARG	A	187	20.997	37.943	51.468	1.00	9.32
2822	NH1	ARG	A	187	19.794	38.386	51.793	1.00	9.21
2825	NH2	ARG	A	187	21.534	36.954	52.172	1.00	8.40
2828	C	ARG	A	187	22.299	43.509	51.635	1.00	8.85
2829	O	ARG	A	187	22.457	42.891	52.686	1.00	8.59
2830	N	PRO	A	188	21.648	44.670	51.567	1.00	9.08
2831	CA	PRO	A	188	21.059	45.291	52.757	1.00	9.34
2833	CB	PRO	A	188	20.270	46.470	52.178	1.00	9.52
2836	CG	PRO	A	188	20.973	46.799	50.913	1.00	9.37
2839	CD	PRO	A	188	21.421	45.483	50.361	1.00	9.02
2842	C	PRO	A	188	20.113	44.346	53.479	1.00	9.61
2843	O	PRO	A	188	19.489	43.509	52.839	1.00	9.17
2844	N	THR	A	189	20.021	44.487	54.797	1.00	10.08
2846	CA	THR	A	189	19.025	43.776	55.585	1.00	10.64
2848	CB	THR	A	189	18.966	44.364	57.002	1.00	10.72
2850	OG1	THR	A	189	20.264	44.306	57.609	1.00	12.49
2852	CG2	THR	A	189	18.091	43.515	57.917	1.00	11.72
2856	C	THR	A	189	17.663	43.923	54.911	1.00	10.69
2857	O	THR	A	189	17.269	45.029	54.564	1.00	10.20

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2858	N	GLY	A	190	16.976	42.805	54.693	1.00	10.96
2860	CA	GLY	A	190	15.627	42.810	54.144	1.00	11.38
2863	C	GLY	A	190	15.556	42.650	52.632	1.00	11.71
2864	O	GLY	A	190	14.465	42.623	52.064	1.00	11.57
2865	N	HIS	A	191	16.714	42.550	51.981	1.00	11.92
2867	CA	HIS	A	191	16.784	42.363	50.534	1.00	12.20
2869	CB	HIS	A	191	17.903	43.220	49.927	1.00	12.31
2872	CG	HIS	A	191	17.491	44.625	49.618	1.00	12.72
2873	ND1	HIS	A	191	17.645	45.186	48.368	1.00	13.27
2875	CE1	HIS	A	191	17.192	46.428	48.387	1.00	13.66
2877	NE2	HIS	A	191	16.761	46.696	49.607	1.00	12.72
2879	CD2	HIS	A	191	16.937	45.585	50.396	1.00	12.96
2881	C	HIS	A	191	17.084	40.895	50.275	1.00	12.38
2882	O	HIS	A	191	18.163	40.434	50.628	1.00	12.13
2883	N	PRO	A	192	16.151	40.148	49.686	1.00	12.83
2884	CA	PRO	A	192	16.416	38.734	49.374	1.00	12.99
2886	CB	PRO	A	192	15.068	38.206	48.856	1.00	13.16
2889	CG	PRO	A	192	14.215	39.396	48.583	1.00	13.46
2892	CD	PRO	A	192	14.791	40.568	49.303	1.00	12.97
2895	C	PRO	A	192	17.534	38.524	48.339	1.00	13.12
2896	O	PRO	A	192	18.205	37.491	48.384	1.00	12.98
2897	N	TYR	A	193	17.723	39.484	47.435	1.00	13.01
2899	CA	TYR	A	193	18.759	39.406	46.404	1.00	13.28
2901	CB	TYR	A	193	18.133	39.481	45.009	1.00	13.73
2904	CG	TYR	A	193	16.960	38.542	44.827	1.00	15.52
2905	CD1	TYR	A	193	15.660	39.031	44.679	1.00	17.56
2907	CE1	TYR	A	193	14.579	38.162	44.519	1.00	18.57
2909	CZ	TYR	A	193	14.800	36.796	44.507	1.00	19.06
2910	OH	TYR	A	193	13.746	35.921	44.351	1.00	20.91
2912	CE2	TYR	A	193	16.081	36.296	44.659	1.00	18.12
2914	CD2	TYR	A	193	17.147	37.167	44.817	1.00	16.56
2916	C	TYR	A	193	19.776	40.532	46.580	1.00	12.67
2917	O	TYR	A	193	19.457	41.566	47.164	1.00	12.10
2918	N	PRO	A	194	20.995	40.345	46.071	1.00	12.36
2919	CA	PRO	A	194	22.033	41.368	46.216	1.00	12.05
2921	CB	PRO	A	194	23.314	40.667	45.730	1.00	12.21
2924	CG	PRO	A	194	22.942	39.263	45.398	1.00	12.23
2927	CD	PRO	A	194	21.475	39.178	45.314	1.00	12.31
2930	C	PRO	A	194	21.765	42.601	45.364	1.00	11.73
2931	O	PRO	A	194	21.135	42.507	44.309	1.00	11.51
2932	N	MSE	A	195	22.211	43.749	45.859	1.00	11.40
2934	CA	MSE	A	195	22.414	44.935	45.039	1.00	11.37
2936	CB	MSE	A	195	22.485	46.182	45.922	1.00	11.37
2939	CG	MSE	A	195	21.212	46.460	46.720	1.00	12.09
2942	SE	MSE	A	195	19.752	47.017	45.570	1.00	13.97
2943	CE	MSE	A	195	20.307	48.880	45.251	1.00	14.52
2947	C	MSE	A	195	23.744	44.737	44.329	1.00	11.09
2948	O	MSE	A	195	24.694	44.251	44.936	1.00	11.00
2949	N	VAL	A	196	23.824	45.088	43.050	1.00	10.94
2951	CA	VAL	A	196	25.066	44.893	42.301	1.00	10.93
2953	CB	VAL	A	196	25.182	43.445	41.716	1.00	11.01
2955	CG1	VAL	A	196	24.035	43.122	40.778	1.00	11.21
2959	CG2	VAL	A	196	26.534	43.241	41.009	1.00	10.99

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2963	C	VAL	A	196	25.261	45.938	41.202	1.00	11.03
2964	O	VAL	A	196	24.341	46.267	40.456	1.00	10.75
2965	N	ASP	A	197	26.477	46.471	41.157	1.00	10.89
2967	CA	ASP	A	197	26.969	47.275	40.055	1.00	10.78
2969	CB	ASP	A	197	27.702	48.500	40.611	1.00	10.72
2972	CG	ASP	A	197	28.136	49.475	39.535	1.00	11.15
2973	OD1	ASP	A	197	28.342	49.052	38.371	1.00	10.48
2974	OD2	ASP	A	197	28.322	50.690	39.778	1.00	9.78
2975	C	ASP	A	197	27.910	46.358	39.278	1.00	10.64
2976	O	ASP	A	197	29.068	46.176	39.658	1.00	10.59
2977	N	GLY	A	198	27.395	45.759	38.208	1.00	10.37
2979	CA	GLY	A	198	28.124	44.766	37.437	1.00	10.19
2982	C	GLY	A	198	29.495	45.234	36.987	1.00	9.97
2983	O	GLY	A	198	30.497	44.590	37.304	1.00	10.01
2984	N	PRO	A	199	29.540	46.327	36.226	1.00	9.78
2985	CA	PRO	A	199	30.807	46.961	35.837	1.00	9.66
2987	CB	PRO	A	199	30.349	48.278	35.211	1.00	9.64
2990	CG	PRO	A	199	29.006	47.957	34.633	1.00	9.92
2993	CD	PRO	A	199	28.380	47.005	35.613	1.00	9.90
2996	C	PRO	A	199	31.772	47.222	36.999	1.00	9.45
2997	O	PRO	A	199	32.940	46.862	36.892	1.00	9.31
2998	N	LEU	A	200	31.290	47.821	38.085	1.00	9.13
3000	CA	LEU	A	200	32.141	48.134	39.235	1.00	9.24
3002	CB	LEU	A	200	31.369	48.946	40.285	1.00	9.17
3005	CG	LEU	A	200	32.048	50.065	41.093	1.00	10.20
3007	CD1	LEU	A	200	31.416	50.193	42.478	1.00	9.79
3011	CD2	LEU	A	200	33.556	49.964	41.198	1.00	10.61
3015	C	LEU	A	200	32.688	46.864	39.883	1.00	8.86
3016	O	LEU	A	200	33.815	46.845	40.353	1.00	8.60
3017	N	SER	A	201	31.877	45.813	39.902	1.00	8.93
3019	CA	SER	A	201	32.258	44.553	40.520	1.00	8.99
3021	CB	SER	A	201	31.037	43.631	40.694	1.00	8.96
3024	OG	SER	A	201	30.650	43.034	39.468	1.00	8.56
3026	C	SER	A	201	33.373	43.876	39.725	1.00	8.97
3027	O	SER	A	201	34.303	43.350	40.313	1.00	8.83
3028	N	ASN	A	202	33.282	43.907	38.397	1.00	9.21
3030	CA	ASN	A	202	34.352	43.395	37.538	1.00	9.42
3032	CB	ASN	A	202	33.968	43.497	36.051	1.00	9.30
3035	CG	ASN	A	202	33.023	42.391	35.591	1.00	10.15
3036	OD1	ASN	A	202	32.700	41.450	36.332	1.00	9.92
3037	ND2	ASN	A	202	32.570	42.505	34.341	1.00	11.15
3040	C	ASN	A	202	35.649	44.170	37.768	1.00	9.26
3041	O	ASN	A	202	36.701	43.577	37.982	1.00	9.22
3042	N	GLU	A	203	35.559	45.495	37.725	1.00	9.43
3044	CA	GLU	A	203	36.728	46.366	37.863	1.00	9.77
3046	CB	GLU	A	203	36.338	47.838	37.641	1.00	10.17
3049	CG	GLU	A	203	37.410	48.875	37.982	1.00	11.47
3052	CD	GLU	A	203	38.661	48.771	37.125	1.00	14.61
3053	OE1	GLU	A	203	38.694	47.939	36.191	1.00	16.44
3054	OE2	GLU	A	203	39.624	49.534	37.386	1.00	15.76
3055	C	GLU	A	203	37.396	46.202	39.220	1.00	9.56
3056	O	GLU	A	203	38.616	46.155	39.306	1.00	9.36
3057	N	THR	A	204	36.588	46.110	40.270	1.00	9.48

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3059	CA	THR	A	204	37.095	46.011	41.631	1.00	9.47
3061	CB	THR	A	204	35.959	46.249	42.661	1.00	9.32
3063	OG1	THR	A	204	35.328	47.516	42.416	1.00	9.28
3065	CG2	THR	A	204	36.519	46.389	44.078	1.00	9.49
3069	C	THR	A	204	37.761	44.655	41.864	1.00	9.32
3070	O	THR	A	204	38.759	44.578	42.568	1.00	9.44
3071	N	TYR	A	205	37.203	43.595	41.279	1.00	9.40
3073	CA	TYR	A	205	37.811	42.263	41.335	1.00	9.27
3075	CB	TYR	A	205	36.919	41.239	40.617	1.00	9.41
3078	CG	TYR	A	205	37.446	39.812	40.598	1.00	9.70
3079	CD1	TYR	A	205	38.587	39.469	39.871	1.00	10.40
3081	CE1	TYR	A	205	39.058	38.167	39.845	1.00	10.53
3083	CZ	TYR	A	205	38.383	37.183	40.543	1.00	10.43
3084	OH	TYR	A	205	38.844	35.893	40.521	1.00	8.84
3086	CE2	TYR	A	205	37.251	37.491	41.264	1.00	10.24
3088	CD2	TYR	A	205	36.783	38.795	41.285	1.00	10.36
3090	C	TYR	A	205	39.199	42.294	40.703	1.00	9.25
3091	O	TYR	A	205	40.171	41.865	41.319	1.00	9.10
3092	N	ILE	A	206	39.279	42.807	39.476	1.00	9.41
3094	CA	ILE	A	206	40.538	42.873	38.735	1.00	9.74
3096	CB	ILE	A	206	40.303	43.384	37.283	1.00	9.65
3098	CG1	ILE	A	206	39.559	42.322	36.467	1.00	9.87
3101	CD1	ILE	A	206	39.022	42.815	35.129	1.00	10.20
3105	CG2	ILE	A	206	41.636	43.746	36.605	1.00	9.77
3109	C	ILE	A	206	41.577	43.736	39.454	1.00	9.91
3110	O	ILE	A	206	42.729	43.328	39.583	1.00	10.17
3111	N	GLN	A	207	41.164	44.912	39.925	1.00	10.11
3113	CA	GLN	A	207	42.070	45.843	40.614	1.00	10.38
3115	CB	GLN	A	207	41.412	47.214	40.806	1.00	10.74
3118	CG	GLN	A	207	41.269	48.027	39.531	1.00	11.84
3121	CD	GLN	A	207	42.598	48.369	38.900	1.00	14.03
3122	OE1	GLN	A	207	42.818	48.099	37.714	1.00	15.97
3123	NE2	GLN	A	207	43.488	48.964	39.681	1.00	14.52
3126	C	GLN	A	207	42.529	45.323	41.971	1.00	10.11
3127	O	GLN	A	207	43.639	45.612	42.391	1.00	10.00
3128	N	SER	A	208	41.670	44.562	42.645	1.00	9.73
3130	CA	SER	A	208	41.999	43.965	43.933	1.00	9.46
3132	CB	ASER	A	208	40.755	43.362	44.592	0.65	9.28
3135	OG	ASER	A	208	39.886	44.380	45.046	0.65	8.22
3137	C	SER	A	208	43.067	42.890	43.767	1.00	9.73
3138	O	SER	A	208	43.988	42.793	44.580	1.00	9.78
3139	N	PHE	A	209	42.945	42.089	42.710	1.00	9.73
3141	CA	PHE	A	209	43.946	41.082	42.409	1.00	9.84
3143	CB	PHE	A	209	43.503	40.147	41.284	1.00	9.83
3146	CG	PHE	A	209	44.606	39.257	40.791	1.00	10.02
3147	CD1	PHE	A	209	45.152	39.431	39.525	1.00	11.34
3149	CE1	PHE	A	209	46.187	38.615	39.082	1.00	11.62
3151	CZ	PHE	A	209	46.694	37.630	39.915	1.00	10.97
3153	CE2	PHE	A	209	46.162	37.455	41.176	1.00	11.11
3155	CD2	PHE	A	209	45.129	38.272	41.614	1.00	10.26
3157	C	PHE	A	209	45.256	41.758	42.025	1.00	9.87
3158	O	PHE	A	209	46.309	41.374	42.505	1.00	9.55
3159	N	ALA	A	210	45.178	42.770	41.167	1.00	10.37

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3161	CA	ALA	A	210	46.357	43.536	40.765	1.00	10.51
3163	CB	ALA	A	210	45.963	44.676	39.822	1.00	10.55
3167	C	ALA	A	210	47.097	44.087	41.983	1.00	10.65
3168	O	ALA	A	210	48.318	44.014	42.053	1.00	10.62
3169	N	GLN	A	211	46.353	44.613	42.951	1.00	10.88
3171	CA	GLN	A	211	46.956	45.238	44.122	1.00	11.24
3173	CB	GLN	A	211	45.920	46.054	44.894	1.00	11.54
3176	CG	GLN	A	211	45.614	47.389	44.244	1.00	13.00
3179	CD	GLN	A	211	44.595	48.181	45.027	1.00	15.10
3180	OE1	GLN	A	211	44.936	48.823	46.019	1.00	16.17
3181	NE2	GLN	A	211	43.341	48.129	44.594	1.00	16.63
3184	C	GLN	A	211	47.639	44.239	45.054	1.00	11.01
3185	O	GLN	A	211	48.768	44.469	45.477	1.00	11.06
3186	N	VAL	A	212	46.965	43.137	45.378	1.00	10.96
3188	CA	VAL	A	212	47.553	42.138	46.277	1.00	10.91
3190	CB	VAL	A	212	46.512	41.141	46.863	1.00	10.99
3192	CG1	VAL	A	212	45.459	41.884	47.697	1.00	10.77
3196	CG2	VAL	A	212	45.859	40.296	45.776	1.00	10.92
3200	C	VAL	A	212	48.690	41.367	45.607	1.00	10.99
3201	O	VAL	A	212	49.643	40.973	46.276	1.00	10.71
3202	N	TRP	A	213	48.586	41.155	44.297	1.00	11.02
3204	CA	TRP	A	213	49.644	40.494	43.539	1.00	11.32
3206	CB	TRP	A	213	49.193	40.147	42.115	1.00	11.16
3209	CG	TRP	A	213	50.333	39.672	41.261	1.00	11.29
3210	CD1	TRP	A	213	51.082	40.423	40.390	1.00	11.41
3212	NE1	TRP	A	213	52.056	39.646	39.811	1.00	11.34
3214	CE2	TRP	A	213	51.957	38.370	40.302	1.00	12.03
3215	CD2	TRP	A	213	50.887	38.353	41.225	1.00	11.82
3216	CE3	TRP	A	213	50.580	37.148	41.872	1.00	12.27
3218	CZ3	TRP	A	213	51.336	36.026	41.589	1.00	12.81
3220	CH2	TRP	A	213	52.393	36.076	40.667	1.00	13.39
3222	CZ2	TRP	A	213	52.715	37.235	40.014	1.00	12.56
3224	C	TRP	A	213	50.896	41.367	43.474	1.00	11.61
3225	O	TRP	A	213	51.997	40.879	43.692	1.00	11.77
3226	N	ASP	A	214	50.720	42.649	43.160	1.00	11.97
3228	CA	ASP	A	214	51.839	43.591	43.073	1.00	12.39
3230	CB	ASP	A	214	51.360	44.985	42.655	1.00	12.46
3233	CG	ASP	A	214	51.026	45.074	41.178	1.00	12.90
3234	OD1	ASP	A	214	50.358	46.055	40.788	1.00	12.70
3235	OD2	ASP	A	214	51.378	44.215	40.340	1.00	14.02
3236	C	ASP	A	214	52.559	43.693	44.411	1.00	12.49
3237	O	ASP	A	214	53.787	43.699	44.461	1.00	12.48
3238	N	GLU	A	215	51.784	43.774	45.487	1.00	12.61
3240	CA	GLU	A	215	52.342	43.863	46.830	1.00	12.87
3242	CB	GLU	A	215	51.258	44.268	47.836	1.00	12.91
3245	CG	GLU	A	215	51.728	44.362	49.286	1.00	13.30
3248	CD	GLU	A	215	52.781	45.435	49.520	1.00	13.66
3249	OE1	GLU	A	215	53.473	45.361	50.556	1.00	14.87
3250	OE2	GLU	A	215	52.916	46.360	48.691	1.00	13.75
3251	C	GLU	A	215	52.995	42.544	47.246	1.00	13.03
3252	O	GLU	A	215	54.001	42.553	47.952	1.00	12.59
3253	N	HIS	A	216	52.424	41.419	46.811	1.00	13.21
3255	CA	HIS	A	216	53.008	40.110	47.095	1.00	13.59

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3257	CB	HIS	A	216	52.081	38.963	46.677	1.00	13.55
3260	CG	HIS	A	216	52.654	37.610	46.961	1.00	13.88
3261	ND1	HIS	A	216	53.566	36.999	46.128	1.00	13.98
3263	CE1	HIS	A	216	53.912	35.831	46.640	1.00	14.60
3265	NE2	HIS	A	216	53.261	35.663	47.777	1.00	13.75
3267	CD2	HIS	A	216	52.473	36.765	48.004	1.00	14.13
3269	C	HIS	A	216	54.359	39.947	46.404	1.00	13.90
3270	O	HIS	A	216	55.289	39.400	46.988	1.00	13.96
3271	N	LYS	A	217	54.461	40.418	45.166	1.00	14.33
3273	CA	LYS	A	217	55.708	40.334	44.408	1.00	14.97
3275	CB	LYS	A	217	55.477	40.707	42.936	1.00	14.97
3278	CG	LYS	A	217	56.744	40.707	42.077	1.00	16.28
3281	CD	LYS	A	217	56.457	41.023	40.617	1.00	17.31
3284	CE	LYS	A	217	57.757	41.163	39.828	1.00	18.89
3287	NZ	LYS	A	217	57.523	41.578	38.410	1.00	19.34
3291	C	LYS	A	217	56.762	41.247	45.042	1.00	15.06
3292	O	LYS	A	217	57.934	40.907	45.077	1.00	14.93
3293	N	LYS	A	218	56.331	42.398	45.551	1.00	15.32
3295	CA	LYS	A	218	57.236	43.355	46.181	1.00	15.67
3297	CB	LYS	A	218	56.491	44.663	46.468	1.00	15.87
3300	CG	LYS	A	218	57.303	45.726	47.187	1.00	16.86
3303	CD	LYS	A	218	56.483	46.990	47.364	1.00	17.91
3306	CE	LYS	A	218	57.215	48.018	48.204	1.00	18.82
3309	NZ	LYS	A	218	56.392	49.250	48.373	1.00	19.84
3313	C	LYS	A	218	57.832	42.776	47.466	1.00	15.60
3314	O	LYS	A	218	59.023	42.932	47.728	1.00	15.45
3315	N	ARG	A	219	57.000	42.092	48.250	1.00	15.60
3317	CA	ARG	A	219	57.422	41.522	49.526	1.00	15.67
3319	CB	ARG	A	219	56.205	41.128	50.367	1.00	15.83
3322	CG	ARG	A	219	55.440	42.292	50.986	1.00	16.43
3325	CD	ARG	A	219	54.271	41.840	51.854	1.00	17.43
3328	NE	ARG	A	219	53.334	42.919	52.166	1.00	18.00
3330	CZ	ARG	A	219	52.237	42.759	52.903	1.00	18.96
3331	NH1	ARG	A	219	51.434	43.792	53.133	1.00	19.57
3334	NH2	ARG	A	219	51.942	41.578	53.426	1.00	19.15
3337	C	ARG	A	219	58.309	40.292	49.353	1.00	15.58
3338	O	ARG	A	219	59.292	40.137	50.073	1.00	15.47
3339	N	THR	A	220	57.960	39.426	48.400	1.00	15.33
3341	CA	THR	A	220	58.542	38.080	48.317	1.00	15.34
3343	CB	THR	A	220	57.423	37.013	48.205	1.00	15.30
3345	OG1	THR	A	220	56.697	37.180	46.974	1.00	15.10
3347	CG2	THR	A	220	56.379	37.181	49.303	1.00	15.04
3351	C	THR	A	220	59.517	37.874	47.159	1.00	15.28
3352	O	THR	A	220	60.326	36.956	47.197	1.00	15.33
3353	N	GLY	A	221	59.419	38.703	46.125	1.00	15.22
3355	CA	GLY	A	221	60.190	38.512	44.909	1.00	15.17
3358	C	GLY	A	221	59.580	37.505	43.941	1.00	15.09
3359	O	GLY	A	221	60.061	37.366	42.821	1.00	15.22
3360	N	LEU	A	222	58.516	36.819	44.357	1.00	14.99
3362	CA	LEU	A	222	57.909	35.763	43.552	1.00	14.90
3364	CB	LEU	A	222	57.062	34.838	44.426	1.00	15.08
3367	CG	LEU	A	222	57.785	34.126	45.577	1.00	15.48
3369	CD1	LEU	A	222	56.775	33.475	46.511	1.00	15.64

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3373	CD2	LEU	A	222	58.783	33.094	45.048	1.00	15.97
3377	C	LEU	A	222	57.059	36.333	42.422	1.00	14.65
3378	O	LEU	A	222	56.424	37.377	42.569	1.00	14.43
3379	N	ASP	A	223	57.054	35.623	41.298	1.00	14.37
3381	CA	ASP	A	223	56.390	36.065	40.074	1.00	14.20
3383	CB	ASP	A	223	57.434	36.669	39.124	1.00	14.31
3386	CG	ASP	A	223	56.868	37.759	38.230	1.00	14.36
3387	OD1	ASP	A	223	57.650	38.642	37.804	1.00	14.98
3388	OD2	ASP	A	223	55.670	37.812	37.887	1.00	13.31
3389	C	ASP	A	223	55.668	34.867	39.440	1.00	14.10
3390	O	ASP	A	223	55.632	33.785	40.025	1.00	13.88
3391	N	PHE	A	224	55.086	35.057	38.258	1.00	14.09
3393	CA	PHE	A	224	54.245	34.033	37.634	1.00	14.25
3395	CB	PHE	A	224	53.601	34.584	36.360	1.00	14.36
3398	CG	PHE	A	224	52.506	35.577	36.625	1.00	14.07
3399	CD1	PHE	A	224	51.260	35.149	37.050	1.00	14.25
3401	CE1	PHE	A	224	50.241	36.066	37.308	1.00	14.53
3403	CZ	PHE	A	224	50.474	37.419	37.143	1.00	14.35
3405	CE2	PHE	A	224	51.716	37.855	36.725	1.00	14.12
3407	CD2	PHE	A	224	52.728	36.936	36.473	1.00	13.93
3409	C	PHE	A	224	54.984	32.721	37.344	1.00	14.39
3410	O	PHE	A	224	54.409	31.638	37.483	1.00	14.36
3411	N	ALA	A	225	56.261	32.824	36.981	1.00	14.50
3413	CA	ALA	A	225	57.093	31.651	36.694	1.00	14.54
3415	CB	ALA	A	225	58.413	32.089	36.054	1.00	14.64
3419	C	ALA	A	225	57.368	30.790	37.934	1.00	14.48
3420	O	ALA	A	225	57.740	29.623	37.811	1.00	14.52
3421	N	ASP	A	226	57.196	31.373	39.120	1.00	14.37
3423	CA	ASP	A	226	57.389	30.660	40.385	1.00	14.29
3425	CB	ASP	A	226	57.828	31.634	41.475	1.00	14.41
3428	CG	ASP	A	226	59.123	32.323	41.137	1.00	14.96
3429	OD1	ASP	A	226	59.161	33.568	41.157	1.00	15.70
3430	OD2	ASP	A	226	60.153	31.695	40.824	1.00	16.10
3431	C	ASP	A	226	56.149	29.903	40.854	1.00	13.93
3432	O	ASP	A	226	56.210	29.180	41.844	1.00	14.19
3433	N	TYR	A	227	55.032	30.068	40.149	1.00	13.69
3435	CA	TYR	A	227	53.790	29.390	40.500	1.00	13.36
3437	CB	TYR	A	227	52.656	30.407	40.648	1.00	13.39
3440	CG	TYR	A	227	52.747	31.099	41.974	1.00	13.55
3441	CD1	TYR	A	227	53.420	32.309	42.103	1.00	13.12
3443	CE1	TYR	A	227	53.536	32.935	43.335	1.00	12.90
3445	CZ	TYR	A	227	52.993	32.336	44.453	1.00	13.21
3446	OH	TYR	A	227	53.108	32.948	45.674	1.00	13.75
3448	CE2	TYR	A	227	52.331	31.125	44.350	1.00	13.04
3450	CD2	TYR	A	227	52.224	30.509	43.120	1.00	13.32
3452	C	TYR	A	227	53.425	28.314	39.493	1.00	13.13
3453	O	TYR	A	227	53.335	28.568	38.300	1.00	12.91
3454	N	ASP	A	228	53.232	27.101	39.993	1.00	13.02
3456	CA	ASP	A	228	52.765	25.990	39.172	1.00	12.87
3458	CB	ASP	A	228	53.015	24.672	39.896	1.00	12.80
3461	CG	ASP	A	228	54.480	24.437	40.149	1.00	12.93
3462	OD1	ASP	A	228	55.158	23.933	39.235	1.00	12.61
3463	OD2	ASP	A	228	55.046	24.755	41.216	1.00	12.06

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3464	C	ASP	A	228	51.286	26.129	38.808	1.00	12.70
3465	O	ASP	A	228	50.850	25.590	37.797	1.00	12.73
3466	N	ALA	A	229	50.524	26.843	39.633	1.00	12.48
3468	CA	ALA	A	229	49.138	27.186	39.306	1.00	12.41
3470	CB	ALA	A	229	48.228	25.971	39.479	1.00	12.51
3474	C	ALA	A	229	48.619	28.351	40.144	1.00	12.35
3475	O	ALA	A	229	49.060	28.559	41.271	1.00	12.18
3476	N	LEU	A	230	47.680	29.101	39.575	1.00	12.14
3478	CA	LEU	A	230	46.977	30.168	40.283	1.00	11.98
3480	CB	LEU	A	230	47.277	31.527	39.662	1.00	12.06
3483	CG	LEU	A	230	48.741	31.962	39.670	1.00	13.01
3485	CD1	LEU	A	230	48.899	33.282	38.919	1.00	13.82
3489	CD2	LEU	A	230	49.261	32.083	41.092	1.00	13.19
3493	C	LEU	A	230	45.474	29.908	40.242	1.00	11.76
3494	O	LEU	A	230	44.875	29.869	39.167	1.00	11.90
3495	N	ALA	A	231	44.885	29.713	41.418	1.00	11.31
3497	CA	ALA	A	231	43.450	29.529	41.571	1.00	11.20
3499	CB	ALA	A	231	43.170	28.412	42.564	1.00	11.34
3503	C	ALA	A	231	42.812	30.837	42.040	1.00	10.96
3504	O	ALA	A	231	43.418	31.598	42.798	1.00	10.56
3505	N	PHE	A	232	41.585	31.078	41.589	1.00	10.56
3507	CA	PHE	A	232	40.882	32.339	41.819	1.00	10.45
3509	CB	PHE	A	232	40.748	33.098	40.499	1.00	10.47
3512	CG	PHE	A	232	42.031	33.711	40.014	1.00	10.95
3513	CD1	PHE	A	232	42.241	35.078	40.112	1.00	11.25
3515	CE1	PHE	A	232	43.423	35.647	39.663	1.00	11.28
3517	CZ	PHE	A	232	44.401	34.853	39.104	1.00	11.30
3519	CE2	PHE	A	232	44.200	33.487	38.990	1.00	11.56
3521	CD2	PHE	A	232	43.020	32.923	39.443	1.00	11.38
3523	C	PHE	A	232	39.481	32.100	42.355	1.00	10.12
3524	O	PHE	A	232	38.896	31.042	42.137	1.00	9.99
3525	N	HIS	A	233	38.927	33.098	43.035	1.00	9.62
3527	CA	HIS	A	233	37.495	33.112	43.300	1.00	9.47
3529	CB	HIS	A	233	37.100	34.360	44.083	1.00	9.43
3532	CG	HIS	A	233	35.625	34.597	44.130	1.00	8.75
3533	ND1	HIS	A	233	34.760	33.757	44.796	1.00	8.36
3535	CE1	HIS	A	233	33.525	34.211	44.666	1.00	8.71
3537	NE2	HIS	A	233	33.559	35.314	43.939	1.00	7.38
3539	CD2	HIS	A	233	34.861	35.578	43.593	1.00	8.29
3541	C	HIS	A	233	36.789	33.108	41.945	1.00	9.39
3542	O	HIS	A	233	37.109	33.932	41.088	1.00	9.26
3543	N	ILE	A	234	35.855	32.177	41.755	1.00	9.28
3545	CA	ILE	A	234	35.147	32.020	40.479	1.00	9.30
3547	CB	ILE	A	234	35.284	30.563	39.943	1.00	9.24
3549	CG1	ILE	A	234	36.753	30.144	39.827	1.00	9.72
3552	CD1	ILE	A	234	36.964	28.640	39.940	1.00	10.24
3556	CG2	ILE	A	234	34.611	30.427	38.577	1.00	9.21
3560	C	ILE	A	234	33.663	32.393	40.590	1.00	9.26
3561	O	ILE	A	234	32.829	31.537	40.867	1.00	9.37
3562	N	PRO	A	235	33.327	33.664	40.369	1.00	9.59
3563	CA	PRO	A	235	31.919	34.084	40.310	1.00	9.73
3565	CB	PRO	A	235	32.002	35.610	40.389	1.00	9.66
3568	CG	PRO	A	235	33.364	35.952	39.856	1.00	9.68

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3571	CD	PRO	A	235	34.251	34.794	40.161	1.00	9.55
3574	C	PRO	A	235	31.265	33.630	39.003	1.00	9.88
3575	O	PRO	A	235	30.095	33.235	38.977	1.00	9.85
3576	N	TYR	A	236	32.039	33.741	37.929	1.00	9.97
3578	CA	TYR	A	236	31.801	33.061	36.661	1.00	10.06
3580	CB	TYR	A	236	30.961	33.919	35.722	1.00	10.08
3583	CG	TYR	A	236	31.461	35.328	35.472	1.00	10.32
3584	CD1	TYR	A	236	32.142	35.643	34.299	1.00	9.99
3586	CE1	TYR	A	236	32.576	36.925	34.040	1.00	10.61
3588	CZ	TYR	A	236	32.329	37.931	34.950	1.00	11.09
3589	OH	TYR	A	236	32.768	39.207	34.671	1.00	12.27
3591	CE2	TYR	A	236	31.641	37.655	36.121	1.00	10.82
3593	CD2	TYR	A	236	31.201	36.357	36.372	1.00	9.99
3595	C	TYR	A	236	33.172	32.757	36.063	1.00	10.28
3596	O	TYR	A	236	34.137	33.442	36.373	1.00	10.16
3597	N	THR	A	237	33.277	31.733	35.222	1.00	10.61
3599	CA	THR	A	237	34.596	31.175	34.915	1.00	11.06
3601	CB	THR	A	237	34.504	29.796	34.217	1.00	10.95
3603	OG1	THR	A	237	33.967	29.940	32.900	1.00	10.27
3605	CG2	THR	A	237	33.540	28.848	34.949	1.00	10.79
3609	C	THR	A	237	35.502	32.110	34.108	1.00	11.63
3610	O	THR	A	237	36.716	31.967	34.155	1.00	11.74
3611	N	LYS	A	238	34.936	33.071	33.392	1.00	12.35
3613	CA	LYS	A	238	35.772	34.020	32.652	1.00	13.33
3615	CB	LYS	A	238	35.032	34.596	31.437	1.00	13.80
3618	CG	LYS	A	238	35.789	34.368	30.125	1.00	16.53
3621	CD	LYS	A	238	34.955	34.768	28.945	1.00	20.06
3624	CE	LYS	A	238	35.652	34.483	27.627	1.00	21.44
3627	NZ	LYS	A	238	35.079	35.333	26.539	1.00	22.72
3631	C	LYS	A	238	36.337	35.146	33.526	1.00	13.19
3632	O	LYS	A	238	37.256	35.836	33.105	1.00	13.23
3633	N	MSE	A	239	35.803	35.332	34.734	1.00	13.14
3635	CA	MSE	A	239	36.278	36.399	35.619	1.00	13.03
3637	CB	MSE	A	239	35.496	36.419	36.938	1.00	13.21
3640	CG	MSE	A	239	35.845	37.601	37.838	1.00	13.27
3643	SE	MSE	A	239	35.184	39.279	37.114	1.00	14.41
3644	CE	MSE	A	239	36.845	40.067	36.493	1.00	13.65
3648	C	MSE	A	239	37.761	36.246	35.921	1.00	13.05
3649	O	MSE	A	239	38.540	37.188	35.744	1.00	12.46
3650	N	GLY	A	240	38.146	35.053	36.365	1.00	12.92
3652	CA	GLY	A	240	39.526	34.775	36.703	1.00	13.08
3655	C	GLY	A	240	40.440	34.951	35.506	1.00	13.30
3656	O	GLY	A	240	41.542	35.481	35.645	1.00	12.94
3657	N	LYS	A	241	39.976	34.520	34.333	1.00	13.29
3659	CA	LYS	A	241	40.747	34.664	33.102	1.00	13.47
3661	CB	LYS	A	241	40.027	34.021	31.905	1.00	13.60
3664	CG	LYS	A	241	40.945	33.808	30.703	1.00	14.20
3667	CD	LYS	A	241	40.193	33.477	29.432	1.00	14.93
3670	CE	LYS	A	241	41.172	33.098	28.320	1.00	15.42
3673	NZ	LYS	A	241	40.489	32.894	27.022	1.00	16.18
3677	C	LYS	A	241	41.041	36.131	32.799	1.00	13.39
3678	O	LYS	A	241	42.151	36.464	32.412	1.00	13.26
3679	N	LYS	A	242	40.042	36.993	32.983	1.00	13.40

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3681	CA	LYS	A	242	40.171	38.422	32.704	1.00	13.29
3683	CB	LYS	A	242	38.796	39.107	32.747	1.00	13.31
3686	CG	LYS	A	242	37.896	38.729	31.573	1.00	13.37
3689	CD	LYS	A	242	36.660	39.606	31.476	1.00	14.18
3692	CE	LYS	A	242	35.626	39.259	32.538	1.00	13.92
3695	NZ	LYS	A	242	34.396	40.094	32.404	1.00	13.37
3699	C	LYS	A	242	41.150	39.108	33.659	1.00	13.17
3700	O	LYS	A	242	41.895	39.990	33.247	1.00	12.84
3701	N	ALA	A	243	41.157	38.688	34.924	1.00	13.18
3703	CA	ALA	A	243	42.105	39.206	35.913	1.00	13.08
3705	CB	ALA	A	243	41.740	38.696	37.299	1.00	13.16
3709	C	ALA	A	243	43.540	38.802	35.561	1.00	13.25
3710	O	ALA	A	243	44.476	39.607	35.666	1.00	12.55
3711	N	LEU	A	244	43.690	37.547	35.140	1.00	13.41
3713	CA	LEU	A	244	44.967	36.993	34.706	1.00	13.76
3715	CB	LEU	A	244	44.807	35.513	34.314	1.00	13.88
3718	CG	LEU	A	244	45.587	34.373	34.987	1.00	13.88
3720	CD1	LEU	A	244	46.371	34.771	36.220	1.00	13.13
3724	CD2	LEU	A	244	44.643	33.210	35.300	1.00	13.61
3728	C	LEU	A	244	45.505	37.773	33.511	1.00	14.11
3729	O	LEU	A	244	46.652	38.202	33.521	1.00	14.01
3730	N	LEU	A	245	44.663	37.967	32.499	1.00	14.45
3732	CA	LEU	A	245	45.059	38.666	31.276	1.00	15.05
3734	CB	LEU	A	245	43.928	38.615	30.236	1.00	15.10
3737	CG	LEU	A	245	43.610	37.239	29.635	1.00	15.53
3739	CD1	LEU	A	245	42.285	37.282	28.882	1.00	16.24
3743	CD2	LEU	A	245	44.719	36.764	28.715	1.00	16.38
3747	C	LEU	A	245	45.475	40.118	31.530	1.00	15.25
3748	O	LEU	A	245	46.306	40.663	30.801	1.00	15.60
3749	N	ALA	A	246	44.915	40.737	32.567	1.00	15.37
3751	CA	ALA	A	246	45.275	42.105	32.934	1.00	15.63
3753	CB	ALA	A	246	44.267	42.664	33.933	1.00	15.62
3757	C	ALA	A	246	46.693	42.224	33.507	1.00	15.85
3758	O	ALA	A	246	47.270	43.311	33.484	1.00	16.08
3759	N	LYS	A	247	47.246	41.123	34.022	1.00	16.04
3761	CA	LYS	A	247	48.539	41.154	34.721	1.00	16.29
3763	CB	LYS	A	247	48.342	40.766	36.195	1.00	16.30
3766	CG	LYS	A	247	47.455	41.722	37.001	1.00	16.75
3769	CD	LYS	A	247	48.035	43.135	37.112	1.00	16.67
3772	CE	LYS	A	247	49.184	43.214	38.101	1.00	16.58
3775	NZ	LYS	A	247	49.942	44.488	37.959	1.00	15.66
3779	C	LYS	A	247	49.668	40.292	34.141	1.00	16.26
3780	O	LYS	A	247	50.814	40.451	34.563	1.00	16.19
3781	N	ILE	A	248	49.371	39.406	33.188	1.00	16.34
3783	CA	ILE	A	248	50.379	38.468	32.670	1.00	16.63
3785	CB	ILE	A	248	49.831	37.009	32.605	1.00	16.58
3787	CG1	ILE	A	248	48.712	36.879	31.559	1.00	16.72
3790	CD1	ILE	A	248	48.431	35.459	31.141	1.00	17.21
3794	CG2	ILE	A	248	49.391	36.534	33.987	1.00	17.19
3798	C	ILE	A	248	50.932	38.847	31.295	1.00	16.60
3799	O	ILE	A	248	51.698	38.084	30.718	1.00	16.44
3800	N	SER	A	249	50.549	40.010	30.774	1.00	16.85
3802	CA	SER	A	249	50.911	40.395	29.407	1.00	17.16

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3804	CB	SER	A	249	50.099	41.617	28.959	1.00	17.16
3807	OG	SER	A	249	50.556	42.797	29.586	1.00	17.71
3809	C	SER	A	249	52.411	40.646	29.202	1.00	17.30
3810	O	SER	A	249	52.890	40.603	28.068	1.00	17.55
3811	N	ASP	A	250	53.145	40.898	30.287	1.00	17.39
3813	CA	ASP	A	250	54.602	41.074	30.224	1.00	17.72
3815	CB	ASP	A	250	55.070	42.078	31.292	1.00	18.24
3818	CG	ASP	A	250	54.888	43.515	30.859	1.00	19.97
3819	OD1	ASP	A	250	55.265	43.843	29.712	1.00	22.70
3820	OD2	ASP	A	250	54.384	44.392	31.597	1.00	23.44
3821	C	ASP	A	250	55.384	39.760	30.378	1.00	17.17
3822	O	ASP	A	250	56.616	39.760	30.329	1.00	17.01
3823	N	GLN	A	251	54.678	38.650	30.570	1.00	16.33
3825	CA	GLN	A	251	55.313	37.335	30.632	1.00	15.93
3827	CB	GLN	A	251	54.441	36.358	31.429	1.00	15.91
3830	CG	GLN	A	251	54.075	36.843	32.832	1.00	15.67
3833	CD	GLN	A	251	55.299	37.163	33.667	1.00	15.80
3834	OE1	GLN	A	251	56.084	36.266	33.985	1.00	16.67
3835	NE2	GLN	A	251	55.476	38.440	34.014	1.00	13.76
3838	C	GLN	A	251	55.570	36.774	29.229	1.00	15.67
3839	O	GLN	A	251	54.943	37.192	28.251	1.00	15.16
3840	N	THR	A	252	56.488	35.816	29.139	1.00	15.50
3842	CA	THR	A	252	56.757	35.129	27.875	1.00	15.52
3844	CB	THR	A	252	57.905	34.103	28.015	1.00	15.54
3846	OG1	THR	A	252	57.499	33.029	28.874	1.00	15.27
3848	CG2	THR	A	252	59.146	34.715	28.708	1.00	15.65
3852	C	THR	A	252	55.490	34.408	27.432	1.00	15.60
3853	O	THR	A	252	54.635	34.095	28.260	1.00	15.29
3854	N	GLU	A	253	55.371	34.148	26.133	1.00	15.70
3856	CA	GLU	A	253	54.202	33.457	25.595	1.00	16.04
3858	CB	GLU	A	253	54.301	33.323	24.067	1.00	16.45
3861	CG	GLU	A	253	53.102	32.656	23.391	1.00	17.80
3864	CD	GLU	A	253	51.777	33.372	23.631	1.00	20.25
3865	OE1	GLU	A	253	51.783	34.605	23.829	1.00	21.15
3866	OE2	GLU	A	253	50.718	32.696	23.608	1.00	21.83
3867	C	GLU	A	253	54.016	32.084	26.244	1.00	15.83
3868	O	GLU	A	253	52.896	31.693	26.549	1.00	15.55
3869	N	ALA	A	254	55.112	31.364	26.467	1.00	15.77
3871	CA	ALA	A	254	55.043	30.040	27.083	1.00	15.57
3873	CB	ALA	A	254	56.411	29.371	27.075	1.00	15.79
3877	C	ALA	A	254	54.490	30.111	28.510	1.00	15.36
3878	O	ALA	A	254	53.695	29.264	28.906	1.00	15.01
3879	N	GLU	A	255	54.908	31.122	29.268	1.00	15.15
3881	CA	GLU	A	255	54.437	31.300	30.645	1.00	15.25
3883	CB	GLU	A	255	55.283	32.340	31.390	1.00	15.32
3886	CG	GLU	A	255	56.695	31.867	31.725	1.00	16.46
3889	CD	GLU	A	255	56.743	30.862	32.863	1.00	17.58
3890	OE1	GLU	A	255	57.834	30.298	33.103	1.00	19.28
3891	OE2	GLU	A	255	55.700	30.629	33.516	1.00	16.76
3892	C	GLU	A	255	52.959	31.695	30.690	1.00	14.93
3893	O	GLU	A	255	52.225	31.224	31.548	1.00	14.65
3894	N	GLN	A	256	52.534	32.551	29.763	1.00	14.88
3896	CA	GLN	A	256	51.129	32.946	29.655	1.00	14.90

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3898	CB	GLN	A	256	50.942	34.028	28.586	1.00	14.83
3901	CG	GLN	A	256	51.620	35.355	28.913	1.00	15.28
3904	CD	GLN	A	256	51.289	36.456	27.915	1.00	15.87
3905	OE1	GLN	A	256	50.140	36.608	27.510	1.00	15.04
3906	NE2	GLN	A	256	52.297	37.229	27.525	1.00	15.87
3909	C	GLN	A	256	50.260	31.738	29.324	1.00	14.97
3910	O	GLN	A	256	49.212	31.537	29.932	1.00	14.79
3911	N	GLU	A	257	50.708	30.927	28.370	1.00	15.15
3913	CA	GLU	A	257	49.942	29.762	27.928	1.00	15.48
3915	CB	GLU	A	257	50.571	29.137	26.674	1.00	15.99
3918	CG	GLU	A	257	50.270	29.899	25.387	1.00	17.00
3921	CD	GLU	A	257	50.813	29.213	24.140	1.00	19.41
3922	OE1	GLU	A	257	50.948	27.966	24.137	1.00	20.60
3923	OE2	GLU	A	257	51.105	29.924	23.150	1.00	20.98
3924	C	GLU	A	257	49.829	28.717	29.040	1.00	15.24
3925	O	GLU	A	257	48.802	28.053	29.170	1.00	15.28
3926	N	ARG	A	258	50.884	28.594	29.844	1.00	14.85
3928	CA	ARG	A	258	50.934	27.630	30.938	1.00	14.84
3930	CB	ARG	A	258	52.374	27.485	31.443	1.00	15.05
3933	CG	ARG	A	258	52.559	26.431	32.519	1.00	15.67
3936	CD	ARG	A	258	53.990	26.334	33.059	1.00	16.97
3939	NE	ARG	A	258	54.412	27.534	33.790	1.00	17.01
3941	CZ	ARG	A	258	53.990	27.877	35.006	1.00	17.70
3942	NH1	ARG	A	258	53.114	27.127	35.659	1.00	17.42
3945	NH2	ARG	A	258	54.443	28.992	35.573	1.00	17.88
3948	C	ARG	A	258	50.022	28.040	32.098	1.00	14.45
3949	O	ARG	A	258	49.338	27.200	32.674	1.00	14.10
3950	N	ILE	A	259	50.026	29.324	32.445	1.00	14.19
3952	CA	ILE	A	259	49.207	29.827	33.550	1.00	14.18
3954	CB	ILE	A	259	49.653	31.258	33.962	1.00	14.35
3956	CG1	ILE	A	259	51.052	31.224	34.588	1.00	14.80
3959	CD1	ILE	A	259	51.095	30.714	36.037	1.00	15.47
3963	CG2	ILE	A	259	48.656	31.888	34.937	1.00	14.33
3967	C	ILE	A	259	47.723	29.795	33.167	1.00	13.92
3968	O	ILE	A	259	46.869	29.466	33.994	1.00	13.64
3969	N	LEU	A	260	47.430	30.113	31.907	1.00	13.67
3971	CA	LEU	A	260	46.056	30.103	31.409	1.00	13.59
3973	CB	LEU	A	260	45.958	30.798	30.047	1.00	13.79
3976	CG	LEU	A	260	46.109	32.320	30.056	1.00	13.94
3978	CD1	LEU	A	260	46.294	32.833	28.640	1.00	14.91
3982	CD2	LEU	A	260	44.915	32.994	30.705	1.00	14.51
3986	C	LEU	A	260	45.509	28.683	31.312	1.00	13.40
3987	O	LEU	A	260	44.322	28.462	31.546	1.00	13.26
3988	N	ALA	A	261	46.376	27.727	30.978	1.00	13.23
3990	CA	ALA	A	261	45.982	26.322	30.876	1.00	12.97
3992	CB	ALA	A	261	47.083	25.498	30.200	1.00	13.22
3996	C	ALA	A	261	45.647	25.741	32.249	1.00	12.72
3997	O	ALA	A	261	44.697	24.966	32.378	1.00	12.45
3998	N	ARG	A	262	46.426	26.109	33.267	1.00	12.25
4000	CA	ARG	A	262	46.125	25.707	34.642	1.00	11.93
4002	CB	ARG	A	262	47.213	26.156	35.622	1.00	11.93
4005	CG	ARG	A	262	48.566	25.499	35.424	1.00	11.69
4008	CD	AARG	A	262	48.600	23.984	35.657	0.65	11.36

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4011	NE	AARG	A	262	48.132	23.231	34.491	0.65	11.38
4013	CZ	AARG	A	262	48.768	23.159	33.320	0.65	10.48
4014	NH1	AARG	A	262	48.236	22.458	32.328	0.65	10.21
4017	NH2	AARG	A	262	49.936	23.759	33.132	0.65	10.36
4020	C	ARG	A	262	44.791	26.291	35.084	1.00	11.78
4021	O	ARG	A	262	44.017	25.621	35.774	1.00	11.46
4022	N	TYR	A	263	44.524	27.536	34.688	1.00	11.46
4024	CA	TYR	A	263	43.266	28.179	35.045	1.00	11.47
4026	CB	TYR	A	263	43.215	29.652	34.609	1.00	11.44
4029	CG	TYR	A	263	41.906	30.284	35.023	1.00	11.19
4030	CD1	TYR	A	263	40.896	30.507	34.097	1.00	11.41
4032	CE1	TYR	A	263	39.679	31.043	34.483	1.00	11.15
4034	CZ	TYR	A	263	39.456	31.347	35.818	1.00	11.66
4035	OH	TYR	A	263	38.250	31.880	36.216	1.00	10.68
4037	CE2	TYR	A	263	40.441	31.117	36.757	1.00	11.14
4039	CD2	TYR	A	263	41.652	30.580	36.358	1.00	11.18
4041	C	TYR	A	263	42.066	27.409	34.476	1.00	11.45
4042	O	TYR	A	263	41.052	27.248	35.159	1.00	11.47
4043	N	GLU	A	264	42.183	26.928	33.240	1.00	11.46
4045	CA	GLU	A	264	41.103	26.158	32.616	1.00	11.61
4047	CB	GLU	A	264	41.455	25.778	31.173	1.00	11.89
4050	CG	GLU	A	264	41.466	26.937	30.192	1.00	12.94
4053	CD	GLU	A	264	40.132	27.656	30.111	1.00	14.36
4054	OE1	GLU	A	264	40.060	28.824	30.552	1.00	15.08
4055	OE2	GLU	A	264	39.157	27.051	29.616	1.00	15.17
4056	C	GLU	A	264	40.774	24.893	33.410	1.00	11.17
4057	O	GLU	A	264	39.614	24.500	33.505	1.00	11.03
4058	N	GLU	A	265	41.799	24.254	33.966	1.00	10.85
4060	CA	GLU	A	265	41.600	23.058	34.783	1.00	10.76
4062	CB	GLU	A	265	42.941	22.383	35.089	1.00	11.00
4065	CG	GLU	A	265	43.543	21.657	33.892	1.00	11.57
4068	CD	GLU	A	265	45.056	21.517	33.955	1.00	12.81
4069	OE1	GLU	A	265	45.678	21.993	34.924	1.00	13.87
4070	OE2	GLU	A	265	45.634	20.927	33.024	1.00	14.57
4071	C	GLU	A	265	40.867	23.392	36.080	1.00	10.42
4072	O	GLU	A	265	40.078	22.587	36.574	1.00	10.42
4073	N	SER	A	266	41.124	24.587	36.611	1.00	9.97
4075	CA	SER	A	266	40.501	25.050	37.848	1.00	9.70
4077	CB	SER	A	266	41.268	26.261	38.416	1.00	9.67
4080	OG	SER	A	266	40.864	27.483	37.816	1.00	9.01
4082	C	SER	A	266	39.012	25.382	37.685	1.00	9.58
4083	O	SER	A	266	38.284	25.399	38.667	1.00	9.63
4084	N	ILE	A	267	38.557	25.627	36.457	1.00	9.58
4086	CA	ILE	A	267	37.149	25.982	36.216	1.00	9.53
4088	CB	ILE	A	267	37.037	27.234	35.290	1.00	9.60
4090	CG1	ILE	A	267	37.700	26.985	33.929	1.00	9.97
4093	CD1	ILE	A	267	37.242	27.939	32.837	1.00	10.63
4097	CG2	ILE	A	267	37.649	28.446	35.970	1.00	9.36
4101	C	ILE	A	267	36.266	24.842	35.681	1.00	9.32
4102	O	ILE	A	267	35.084	25.051	35.445	1.00	9.48
4103	N	VAL	A	268	36.820	23.644	35.515	1.00	9.59
4105	CA	VAL	A	268	36.061	22.513	34.971	1.00	9.51
4107	CB	VAL	A	268	36.902	21.213	34.945	1.00	9.57

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4109	CG1	VAL	A	268	36.040	20.005	34.544	1.00	10.02
4113	CG2	VAL	A	268	38.091	21.361	33.987	1.00	9.79
4117	C	VAL	A	268	34.755	22.279	35.748	1.00	9.45
4118	O	VAL	A	268	33.679	22.215	35.148	1.00	9.60
4119	N	TYR	A	269	34.848	22.171	37.072	1.00	9.19
4121	CA	TYR	A	269	33.670	21.926	37.907	1.00	9.07
4123	CB	TYR	A	269	34.074	21.504	39.329	1.00	9.21
4126	CG	TYR	A	269	34.731	20.135	39.459	1.00	9.43
4127	CD1	TYR	A	269	35.500	19.824	40.578	1.00	10.23
4129	CE1	TYR	A	269	36.105	18.576	40.717	1.00	9.75
4131	CZ	TYR	A	269	35.938	17.621	39.732	1.00	9.77
4132	OH	TYR	A	269	36.534	16.387	39.866	1.00	9.83
4134	CE2	TYR	A	269	35.178	17.902	38.614	1.00	9.59
4136	CD2	TYR	A	269	34.578	19.148	38.481	1.00	9.81
4138	C	TYR	A	269	32.743	23.144	37.969	1.00	9.12
4139	O	TYR	A	269	31.517	22.996	37.951	1.00	8.85
4140	N	SER	A	270	33.327	24.341	38.029	1.00	8.95
4142	CA	SER	A	270	32.549	25.580	38.119	1.00	9.04
4144	CB	ASER	A	270	33.463	26.800	38.285	0.65	8.83
4147	OG	ASER	A	270	33.873	26.944	39.631	0.65	8.28
4149	C	SER	A	270	31.645	25.772	36.903	1.00	9.50
4150	O	SER	A	270	30.571	26.355	37.018	1.00	9.48
4151	N	ARG	A	271	32.073	25.269	35.746	1.00	9.75
4153	CA	ARG	A	271	31.258	25.337	34.535	1.00	10.20
4155	CB	ARG	A	271	32.033	24.822	33.319	1.00	10.52
4158	CG	ARG	A	271	33.219	25.682	32.902	1.00	12.04
4161	CD	ARG	A	271	33.860	25.233	31.593	1.00	14.32
4164	NE	ARG	A	271	32.938	25.434	30.477	1.00	16.57
4166	CZ	ARG	A	271	32.807	26.571	29.793	1.00	17.38
4167	NH1	ARG	A	271	33.573	27.625	30.048	1.00	18.13
4170	NH2	ARG	A	271	31.905	26.645	28.826	1.00	18.27
4173	C	ARG	A	271	29.969	24.530	34.689	1.00	9.90
4174	O	ARG	A	271	29.004	24.782	33.990	1.00	9.82
4175	N	ARG	A	272	29.969	23.553	35.593	1.00	9.79
4177	CA	ARG	A	272	28.801	22.707	35.834	1.00	9.64
4179	CB	ARG	A	272	29.247	21.250	35.950	1.00	9.58
4182	CG	ARG	A	272	30.072	20.753	34.776	1.00	10.52
4185	CD	ARG	A	272	30.495	19.301	34.917	1.00	11.34
4188	NE	ARG	A	272	29.333	18.410	34.908	1.00	11.95
4190	CZ	ARG	A	272	29.371	17.113	35.195	1.00	13.18
4191	NH1	ARG	A	272	30.513	16.516	35.523	1.00	13.54
4194	NH2	ARG	A	272	28.252	16.402	35.148	1.00	13.69
4197	C	ARG	A	272	27.990	23.090	37.081	1.00	9.50
4198	O	ARG	A	272	26.998	22.438	37.388	1.00	9.30
4199	N	VAL	A	273	28.386	24.156	37.774	1.00	9.32
4201	CA	VAL	A	273	27.826	24.484	39.089	1.00	9.24
4203	CB	VAL	A	273	28.836	24.123	40.196	1.00	9.06
4205	CG1	VAL	A	273	28.420	24.710	41.546	1.00	9.50
4209	CG2	VAL	A	273	28.980	22.606	40.291	1.00	9.79
4213	C	VAL	A	273	27.424	25.953	39.217	1.00	9.00
4214	O	VAL	A	273	26.290	26.261	39.587	1.00	8.83
4215	N	GLY	A	274	28.365	26.849	38.936	1.00	8.89
4217	CA	GLY	A	274	28.133	28.281	39.022	1.00	8.88

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4220	C	GLY	A	274	28.753	28.841	40.286	1.00	8.84
4221	O	GLY	A	274	29.564	28.175	40.930	1.00	8.79
4222	N	ASN	A	275	28.362	30.061	40.645	1.00	8.87
4224	CA	ASN	A	275	28.916	30.746	41.812	1.00	8.85
4226	CB	ASN	A	275	28.529	32.235	41.792	1.00	8.70
4229	CG	ASN	A	275	29.463	33.115	42.622	1.00	8.94
4230	OD1	ASN	A	275	30.262	32.625	43.425	1.00	8.05
4231	ND2	ASN	A	275	29.361	34.437	42.424	1.00	7.58
4234	C	ASN	A	275	28.450	30.093	43.119	1.00	8.92
4235	O	ASN	A	275	27.251	29.995	43.380	1.00	8.75
4236	N	LEU	A	276	29.414	29.644	43.921	1.00	9.21
4238	CA	LEU	A	276	29.176	29.155	45.282	1.00	9.50
4240	CB	LEU	A	276	30.065	27.934	45.569	1.00	9.87
4243	CG	LEU	A	276	29.846	26.664	44.750	1.00	11.31
4245	CD1	LEU	A	276	30.542	25.486	45.425	1.00	12.59
4249	CD2	LEU	A	276	28.376	26.373	44.601	1.00	12.44
4253	C	LEU	A	276	29.486	30.233	46.325	1.00	9.08
4254	O	LEU	A	276	29.597	29.935	47.514	1.00	8.62
4255	N	TYR	A	277	29.593	31.481	45.874	1.00	8.74
4257	CA	TYR	A	277	30.076	32.597	46.689	1.00	8.39
4259	CB	TYR	A	277	28.962	33.122	47.617	1.00	8.37
4262	CG	TYR	A	277	27.861	33.966	46.969	1.00	8.51
4263	CD1	TYR	A	277	28.043	34.605	45.739	1.00	8.90
4265	CE1	TYR	A	277	27.033	35.382	45.172	1.00	8.79
4267	CZ	TYR	A	277	25.827	35.521	45.826	1.00	8.70
4268	OH	TYR	A	277	24.829	36.282	45.262	1.00	9.50
4270	CE2	TYR	A	277	25.618	34.898	47.042	1.00	8.82
4272	CD2	TYR	A	277	26.631	34.126	47.606	1.00	8.40
4274	C	TYR	A	277	31.363	32.254	47.474	1.00	8.10
4275	O	TYR	A	277	32.440	32.175	46.879	1.00	8.20
4276	N	THR	A	278	31.265	32.054	48.790	1.00	7.83
4278	CA	THR	A	278	32.447	31.790	49.619	1.00	7.68
4280	CB	THR	A	278	32.081	31.570	51.110	1.00	7.53
4282	OG1	THR	A	278	31.009	30.624	51.226	1.00	6.29
4284	CG2	THR	A	278	31.566	32.858	51.771	1.00	7.58
4288	C	THR	A	278	33.214	30.568	49.135	1.00	7.95
4289	O	THR	A	278	34.437	30.517	49.241	1.00	8.42
4290	N	GLY	A	279	32.481	29.585	48.621	1.00	8.08
4292	CA	GLY	A	279	33.049	28.320	48.204	1.00	8.20
4295	C	GLY	A	279	33.725	28.289	46.848	1.00	8.28
4296	O	GLY	A	279	34.439	27.334	46.570	1.00	8.35
4297	N	SER	A	280	33.532	29.316	46.020	1.00	8.21
4299	CA	SER	A	280	33.980	29.271	44.623	1.00	8.21
4301	CB	SER	A	280	33.554	30.532	43.873	1.00	8.03
4304	OG	SER	A	280	32.147	30.651	43.841	1.00	8.53
4306	C	SER	A	280	35.482	29.067	44.443	1.00	8.10
4307	O	SER	A	280	35.895	28.262	43.611	1.00	7.89
4308	N	LEU	A	281	36.288	29.812	45.200	1.00	8.23
4310	CA	LEU	A	281	37.746	29.672	45.166	1.00	8.11
4312	CB	LEU	A	281	38.425	30.620	46.168	1.00	8.18
4315	CG	LEU	A	281	39.923	30.393	46.441	1.00	8.38
4317	CD1	LEU	A	281	40.747	30.579	45.174	1.00	8.36
4321	CD2	LEU	A	281	40.437	31.313	47.538	1.00	8.23

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4325	C	LEU	A	281	38.147	28.240	45.484	1.00	8.25
4326	O	LEU	A	281	39.031	27.676	44.843	1.00	7.91
4327	N	TYR	A	282	37.489	27.662	46.481	1.00	8.36
4329	CA	TYR	A	282	37.851	26.337	46.972	1.00	8.55
4331	CB	TYR	A	282	37.457	26.212	48.452	1.00	8.56
4334	CG	TYR	A	282	38.166	27.302	49.215	1.00	9.12
4335	CD1	TYR	A	282	39.547	27.244	49.396	1.00	9.10
4337	CE1	TYR	A	282	40.231	28.258	50.029	1.00	9.11
4339	CZ	TYR	A	282	39.548	29.372	50.473	1.00	8.49
4340	OH	TYR	A	282	40.256	30.364	51.101	1.00	9.74
4342	CE2	TYR	A	282	38.176	29.479	50.287	1.00	8.84
4344	CD2	TYR	A	282	37.493	28.449	49.641	1.00	9.17
4346	C	TYR	A	282	37.329	25.212	46.075	1.00	8.52
4347	O	TYR	A	282	37.946	24.157	46.000	1.00	8.50
4348	N	LEU	A	283	36.237	25.455	45.356	1.00	8.61
4350	CA	LEU	A	283	35.784	24.528	44.324	1.00	8.58
4352	CB	LEU	A	283	34.409	24.928	43.777	1.00	8.52
4355	CG	LEU	A	283	33.858	24.075	42.627	1.00	8.62
4357	CD1	LEU	A	283	33.607	22.644	43.087	1.00	8.94
4361	CD2	LEU	A	283	32.573	24.690	42.056	1.00	8.73
4365	C	LEU	A	283	36.812	24.524	43.202	1.00	8.52
4366	O	LEU	A	283	37.115	23.481	42.637	1.00	8.44
4367	N	GLY	A	284	37.355	25.698	42.896	1.00	8.64
4369	CA	GLY	A	284	38.396	25.818	41.898	1.00	8.70
4372	C	GLY	A	284	39.663	25.077	42.282	1.00	8.71
4373	O	GLY	A	284	40.315	24.495	41.422	1.00	8.58
4374	N	LEU	A	285	40.008	25.091	43.568	1.00	8.84
4376	CA	LEU	A	285	41.163	24.346	44.060	1.00	8.71
4378	CB	LEU	A	285	41.435	24.656	45.535	1.00	8.87
4381	CG	LEU	A	285	42.538	23.833	46.214	1.00	8.94
4383	CD1	LEU	A	285	43.886	24.050	45.535	1.00	9.39
4387	CD2	LEU	A	285	42.623	24.168	47.683	1.00	8.77
4391	C	LEU	A	285	40.941	22.851	43.872	1.00	8.67
4392	O	LEU	A	285	41.832	22.147	43.404	1.00	8.45
4393	N	ILE	A	286	39.752	22.374	44.232	1.00	8.66
4395	CA	ILE	A	286	39.410	20.958	44.072	1.00	8.64
4397	CB	ILE	A	286	37.997	20.654	44.632	1.00	8.70
4399	CG1	ILE	A	286	37.943	20.852	46.148	1.00	9.02
4402	CD1	ILE	A	286	36.532	20.771	46.708	1.00	9.27
4406	CG2	ILE	A	286	37.583	19.224	44.278	1.00	9.03
4410	C	ILE	A	286	39.444	20.570	42.594	1.00	8.40
4411	O	ILE	A	286	39.951	19.509	42.230	1.00	8.45
4412	N	SER	A	287	38.883	21.428	41.752	1.00	8.38
4414	CA	SER	A	287	38.788	21.160	40.322	1.00	8.50
4416	CB	SER	A	287	37.970	22.245	39.621	1.00	8.63
4419	OG	SER	A	287	37.865	21.986	38.228	1.00	8.70
4421	C	SER	A	287	40.178	21.085	39.713	1.00	8.70
4422	O	SER	A	287	40.451	20.222	38.876	1.00	8.70
4423	N	LEU	A	288	41.055	21.979	40.155	1.00	8.70
4425	CA	LEU	A	288	42.425	22.024	39.681	1.00	9.02
4427	CB	LEU	A	288	43.173	23.189	40.334	1.00	9.08
4430	CG	LEU	A	288	44.664	23.318	40.020	1.00	9.63
4432	CD1	LEU	A	288	44.880	23.628	38.541	1.00	9.47

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4436	CD2	LEU	A	288	45.284	24.389	40.904	1.00	10.42
4440	C	LEU	A	288	43.135	20.711	39.989	1.00	9.00
4441	O	LEU	A	288	43.756	20.120	39.115	1.00	8.91
4442	N	LEU	A	289	43.031	20.254	41.232	1.00	9.02
4444	CA	LEU	A	289	43.750	19.059	41.665	1.00	9.24
4446	CB	LEU	A	289	43.780	18.966	43.193	1.00	9.31
4449	CG	LEU	A	289	44.371	20.182	43.921	1.00	9.40
4451	CD1	LEU	A	289	44.594	19.863	45.377	1.00	9.52
4455	CD2	LEU	A	289	45.671	20.678	43.276	1.00	9.44
4459	C	LEU	A	289	43.166	17.785	41.071	1.00	9.34
4460	O	LEU	A	289	43.903	16.839	40.820	1.00	9.59
4461	N	GLU	A	290	41.857	17.765	40.825	1.00	9.47
4463	CA	GLU	A	290	41.193	16.559	40.319	1.00	9.89
4465	CB	GLU	A	290	39.779	16.424	40.910	1.00	9.82
4468	CG	GLU	A	290	39.822	15.948	42.354	1.00	9.67
4471	CD	GLU	A	290	38.479	15.927	43.059	1.00	10.11
4472	OE1	GLU	A	290	37.433	16.076	42.401	1.00	9.35
4473	OE2	GLU	A	290	38.478	15.756	44.299	1.00	9.95
4474	C	GLU	A	290	41.178	16.476	38.791	1.00	10.33
4475	O	GLU	A	290	40.897	15.414	38.233	1.00	10.92
4476	N	ASN	A	291	41.521	17.572	38.115	1.00	10.64
4478	CA	ASN	A	291	41.537	17.598	36.650	1.00	11.20
4480	CB	ASN	A	291	40.564	18.658	36.125	1.00	10.92
4483	CG	ASN	A	291	39.116	18.277	36.353	1.00	11.08
4484	OD1	ASN	A	291	38.585	17.389	35.676	1.00	10.76
4485	ND2	ASN	A	291	38.464	18.940	37.314	1.00	9.82
4488	C	ASN	A	291	42.924	17.789	36.022	1.00	11.68
4489	O	ASN	A	291	43.101	17.535	34.831	1.00	12.13
4490	N	ALA	A	292	43.904	18.223	36.810	1.00	12.16
4492	CA	ALA	A	292	45.266	18.396	36.308	1.00	12.58
4494	CB	ALA	A	292	46.092	19.220	37.277	1.00	12.39
4498	C	ALA	A	292	45.928	17.037	36.070	1.00	12.93
4499	O	ALA	A	292	45.578	16.044	36.714	1.00	13.31
4500	N	THR	A	293	46.862	16.995	35.125	1.00	13.24
4502	CA	THR	A	293	47.683	15.806	34.898	1.00	13.57
4504	CB	THR	A	293	47.458	15.261	33.474	1.00	13.57
4506	OG1	THR	A	293	47.817	16.253	32.502	1.00	13.65
4508	CG2	THR	A	293	45.967	14.995	33.213	1.00	13.56
4512	C	THR	A	293	49.181	16.042	35.136	1.00	13.82
4513	O	THR	A	293	49.942	15.075	35.216	1.00	14.12
4514	N	THR	A	294	49.597	17.307	35.264	1.00	13.87
4516	CA	THR	A	294	51.015	17.664	35.405	1.00	13.84
4518	CB	THR	A	294	51.447	18.646	34.290	1.00	14.00
4520	OG1	THR	A	294	50.733	19.879	34.416	1.00	13.79
4522	CG2	THR	A	294	51.068	18.131	32.905	1.00	14.47
4526	C	THR	A	294	51.382	18.275	36.767	1.00	13.69
4527	O	THR	A	294	52.557	18.566	37.014	1.00	13.89
4528	N	LEU	A	295	50.399	18.482	37.640	1.00	13.12
4530	CA	LEU	A	295	50.688	18.908	39.005	1.00	12.78
4532	CB	LEU	A	295	49.449	19.513	39.673	1.00	12.73
4535	CG	LEU	A	295	48.997	20.871	39.137	1.00	12.56
4537	CD1	LEU	A	295	50.092	21.924	39.292	1.00	12.76
4541	CD2	LEU	A	295	47.723	21.316	39.835	1.00	12.97

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4545	C	LEU	A	295	51.214	17.728	39.825	1.00	12.71
4546	O	LEU	A	295	50.805	16.579	39.630	1.00	12.26
4547	N	THR	A	296	52.121	18.030	40.747	1.00	12.72
4549	CA	THR	A	296	52.761	17.021	41.578	1.00	12.77
4551	CB	THR	A	296	53.936	16.365	40.799	1.00	13.01
4553	OG1	THR	A	296	54.442	15.242	41.528	1.00	13.56
4555	CG2	THR	A	296	55.137	17.304	40.674	1.00	13.30
4559	C	THR	A	296	53.234	17.621	42.902	1.00	12.58
4560	O	THR	A	296	53.312	18.843	43.049	1.00	12.37
4561	N	ALA	A	297	53.533	16.753	43.863	1.00	12.15
4563	CA	ALA	A	297	54.014	17.173	45.181	1.00	12.17
4565	CB	ALA	A	297	54.411	15.953	46.004	1.00	12.24
4569	C	ALA	A	297	55.192	18.137	45.074	1.00	12.03
4570	O	ALA	A	297	56.084	17.944	44.246	1.00	11.87
4571	N	GLY	A	298	55.176	19.179	45.902	1.00	11.72
4573	CA	GLY	A	298	56.208	20.203	45.893	1.00	11.69
4576	C	GLY	A	298	55.806	21.457	45.135	1.00	11.49
4577	O	GLY	A	298	56.389	22.521	45.352	1.00	11.72
4578	N	ASN	A	299	54.816	21.334	44.252	1.00	11.26
4580	CA	ASN	A	299	54.354	22.449	43.422	1.00	11.14
4582	CB	ASN	A	299	53.321	21.976	42.383	1.00	10.93
4585	CG	ASN	A	299	53.940	21.226	41.194	1.00	11.89
4586	OD1	ASN	A	299	53.210	20.785	40.302	1.00	12.20
4587	ND2	ASN	A	299	55.267	21.084	41.170	1.00	11.78
4590	C	ASN	A	299	53.725	23.558	44.268	1.00	10.95
4591	O	ASN	A	299	53.098	23.287	45.295	1.00	10.82
4592	N	GLN	A	300	53.893	24.801	43.820	1.00	10.62
4594	CA	GLN	A	300	53.370	25.978	44.503	1.00	10.59
4596	CB	GLN	A	300	54.389	27.125	44.450	1.00	10.64
4599	CG	GLN	A	300	55.800	26.744	44.912	1.00	10.75
4602	CD	GLN	A	300	55.848	26.350	46.372	1.00	10.79
4603	OE1	GLN	A	300	55.566	27.168	47.250	1.00	11.66
4604	NE2	GLN	A	300	56.205	25.102	46.640	1.00	10.15
4607	C	GLN	A	300	52.060	26.429	43.860	1.00	10.45
4608	O	GLN	A	300	52.006	26.662	42.655	1.00	10.12
4609	N	ILE	A	301	51.012	26.531	44.675	1.00	10.19
4611	CA	ILE	A	301	49.695	26.983	44.244	1.00	10.27
4613	CB	ILE	A	301	48.601	25.960	44.671	1.00	10.29
4615	CG1	ILE	A	301	49.012	24.522	44.319	1.00	10.32
4618	CD1	ILE	A	301	49.292	24.282	42.841	1.00	10.76
4622	CG2	ILE	A	301	47.264	26.303	44.035	1.00	10.38
4626	C	ILE	A	301	49.404	28.335	44.882	1.00	10.08
4627	O	ILE	A	301	49.353	28.444	46.103	1.00	9.85
4628	N	GLY	A	302	49.244	29.368	44.063	1.00	9.94
4630	CA	GLY	A	302	48.768	30.654	44.535	1.00	9.95
4633	C	GLY	A	302	47.250	30.694	44.527	1.00	9.87
4634	O	GLY	A	302	46.619	30.141	43.634	1.00	9.95
4635	N	LEU	A	303	46.666	31.361	45.514	1.00	9.87
4637	CA	LEU	A	303	45.217	31.467	45.639	1.00	9.75
4639	CB	LEU	A	303	44.718	30.632	46.814	1.00	10.07
4642	CG	LEU	A	303	44.939	29.121	46.714	1.00	10.40
4644	CD1	LEU	A	303	46.155	28.711	47.502	1.00	11.23
4648	CD2	LEU	A	303	43.718	28.365	47.206	1.00	11.26

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4652	C	LEU	A	303	44.815	32.916	45.852	1.00	9.66
4653	O	LEU	A	303	45.345	33.577	46.737	1.00	9.54
4654	N	PHE	A	304	43.877	33.397	45.038	1.00	9.37
4656	CA	PHE	A	304	43.315	34.733	45.181	1.00	9.15
4658	CB	PHE	A	304	43.346	35.488	43.852	1.00	9.07
4661	CG	PHE	A	304	42.619	36.804	43.900	1.00	8.84
4662	CD1	PHE	A	304	41.452	37.000	43.176	1.00	9.28
4664	CE1	PHE	A	304	40.781	38.216	43.228	1.00	9.27
4666	CZ	PHE	A	304	41.271	39.243	44.020	1.00	8.92
4668	CE2	PHE	A	304	42.424	39.053	44.750	1.00	9.41
4670	CD2	PHE	A	304	43.090	37.835	44.693	1.00	9.35
4672	C	PHE	A	304	41.873	34.641	45.647	1.00	8.91
4673	O	PHE	A	304	41.011	34.139	44.916	1.00	8.83
4674	N	SER	A	305	41.617	35.111	46.866	1.00	8.69
4676	CA	SER	A	305	40.268	35.189	47.405	1.00	8.71
4678	CB	SER	A	305	40.250	34.761	48.872	1.00	8.91
4681	OG	SER	A	305	38.925	34.760	49.378	1.00	8.85
4683	C	SER	A	305	39.745	36.615	47.282	1.00	8.74
4684	O	SER	A	305	40.464	37.575	47.560	1.00	8.40
4685	N	TYR	A	306	38.495	36.746	46.854	1.00	8.84
4687	CA	TYR	A	306	37.836	38.042	46.776	1.00	8.90
4689	CB	TYR	A	306	37.658	38.473	45.315	1.00	9.03
4692	CG	TYR	A	306	36.989	39.829	45.150	1.00	8.97
4693	CD1	TYR	A	306	35.622	39.930	44.890	1.00	9.44
4695	CE1	TYR	A	306	35.005	41.169	44.741	1.00	9.01
4697	CZ	TYR	A	306	35.757	42.327	44.845	1.00	9.46
4698	OH	TYR	A	306	35.154	43.564	44.693	1.00	9.46
4700	CE2	TYR	A	306	37.117	42.251	45.096	1.00	9.35
4702	CD2	TYR	A	306	37.725	41.008	45.248	1.00	9.15
4704	C	TYR	A	306	36.476	38.003	47.457	1.00	9.03
4705	O	TYR	A	306	35.757	37.008	47.389	1.00	8.97
4706	N	GLY	A	307	36.139	39.113	48.103	1.00	8.79
4708	CA	GLY	A	307	34.822	39.338	48.658	1.00	8.63
4711	C	GLY	A	307	34.418	40.763	48.335	1.00	8.73
4712	O	GLY	A	307	35.178	41.699	48.577	1.00	8.53
4713	N	SER	A	308	33.230	40.933	47.769	1.00	8.82
4715	CA	SER	A	308	32.736	42.255	47.414	1.00	8.77
4717	CB	SER	A	308	31.406	42.145	46.676	1.00	8.84
4720	OG	SER	A	308	31.615	41.873	45.297	1.00	9.01
4722	C	SER	A	308	32.585	43.092	48.680	1.00	8.82
4723	O	SER	A	308	32.346	42.548	49.759	1.00	8.61
4724	N	GLY	A	309	32.771	44.407	48.564	1.00	8.95
4726	CA	GLY	A	309	32.613	45.286	49.709	1.00	9.08
4729	C	GLY	A	309	33.721	46.267	50.073	1.00	9.19
4730	O	GLY	A	309	33.384	47.328	50.599	1.00	9.59
4731	N	ALA	A	310	35.010	45.979	49.856	1.00	9.12
4733	CA	ALA	A	310	35.550	44.743	49.295	1.00	9.06
4735	CB	ALA	A	310	35.854	44.925	47.801	1.00	9.22
4739	C	ALA	A	310	36.828	44.338	50.028	1.00	8.95
4740	O	ALA	A	310	37.618	45.190	50.435	1.00	8.64
4741	N	VAL	A	311	37.023	43.032	50.184	1.00	8.73
4743	CA	VAL	A	311	38.198	42.476	50.842	1.00	8.86
4745	CB	VAL	A	311	37.814	41.884	52.209	1.00	8.75

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4747	CG1	VAL	A	311	39.012	41.211	52.890	1.00	8.70
4751	CG2	VAL	A	311	37.218	42.978	53.098	1.00	8.85
4755	C	VAL	A	311	38.815	41.393	49.957	1.00	8.91
4756	O	VAL	A	311	38.101	40.587	49.380	1.00	9.22
4757	N	ALA	A	312	40.137	41.381	49.843	1.00	9.19
4759	CA	ALA	A	312	40.828	40.345	49.078	1.00	9.12
4761	CB	ALA	A	312	41.156	40.854	47.689	1.00	9.15
4765	C	ALA	A	312	42.095	39.864	49.773	1.00	9.28
4766	O	ALA	A	312	42.601	40.509	50.680	1.00	9.01
4767	N	GLU	A	313	42.599	38.716	49.333	1.00	9.43
4769	CA	GLU	A	313	43.807	38.133	49.895	1.00	9.80
4771	CB	GLU	A	313	43.487	37.380	51.187	1.00	9.88
4774	CG	GLU	A	313	44.692	36.701	51.835	1.00	11.08
4777	CD	GLU	A	313	44.442	36.289	53.277	1.00	12.23
4778	OE1	GLU	A	313	43.392	36.658	53.841	1.00	14.20
4779	OE2	GLU	A	313	45.304	35.602	53.855	1.00	13.22
4780	C	GLU	A	313	44.459	37.184	48.900	1.00	9.80
4781	O	GLU	A	313	43.787	36.336	48.314	1.00	9.64
4782	N	PHE	A	314	45.762	37.347	48.701	1.00	9.72
4784	CA	PHE	A	314	46.558	36.375	47.975	1.00	9.99
4786	CB	PHE	A	314	47.469	37.068	46.970	1.00	9.90
4789	CG	PHE	A	314	48.222	36.117	46.093	1.00	10.55
4790	CD1	PHE	A	314	47.625	35.579	44.960	1.00	10.91
4792	CE1	PHE	A	314	48.316	34.696	44.146	1.00	11.38
4794	CZ	PHE	A	314	49.613	34.334	44.467	1.00	11.49
4796	CE2	PHE	A	314	50.215	34.853	45.593	1.00	11.30
4798	CD2	PHE	A	314	49.519	35.741	46.406	1.00	11.26
4800	C	PHE	A	314	47.390	35.579	48.970	1.00	10.10
4801	O	PHE	A	314	47.962	36.144	49.897	1.00	10.31
4802	N	PHE	A	315	47.454	34.266	48.782	1.00	10.34
4804	CA	PHE	A	315	48.241	33.399	49.655	1.00	10.44
4806	CB	PHE	A	315	47.489	33.107	50.964	1.00	10.61
4809	CG	PHE	A	315	46.206	32.328	50.788	1.00	11.09
4810	CD1	PHE	A	315	46.170	30.957	51.021	1.00	10.66
4812	CE1	PHE	A	315	44.985	30.238	50.870	1.00	10.90
4814	CZ	PHE	A	315	43.823	30.891	50.494	1.00	11.17
4816	CE2	PHE	A	315	43.844	32.260	50.268	1.00	11.22
4818	CD2	PHE	A	315	45.029	32.971	50.414	1.00	11.10
4820	C	PHE	A	315	48.629	32.113	48.935	1.00	10.60
4821	O	PHE	A	315	48.031	31.753	47.921	1.00	10.36
4822	N	THR	A	316	49.637	31.424	49.458	1.00	10.78
4824	CA	THR	A	316	50.228	30.281	48.768	1.00	11.04
4826	CB	THR	A	316	51.713	30.574	48.453	1.00	11.21
4828	OG1	THR	A	316	51.809	31.721	47.596	1.00	12.11
4830	CG2	THR	A	316	52.347	29.450	47.630	1.00	11.83
4834	C	THR	A	316	50.111	28.994	49.578	1.00	11.02
4835	O	THR	A	316	50.136	29.013	50.807	1.00	10.73
4836	N	GLY	A	317	49.966	27.883	48.863	1.00	10.94
4838	CA	GLY	A	317	50.042	26.551	49.429	1.00	11.14
4841	C	GLY	A	317	50.988	25.690	48.609	1.00	11.32
4842	O	GLY	A	317	51.249	25.973	47.439	1.00	11.78
4843	N	GLU	A	318	51.518	24.643	49.227	1.00	11.12
4845	CA	GLU	A	318	52.373	23.690	48.541	1.00	11.00

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4847	CB	GLU	A	318	53.732	23.594	49.240	1.00	11.07
4850	CG	GLU	A	318	54.680	22.563	48.645	1.00	11.58
4853	CD	GLU	A	318	56.074	22.639	49.235	1.00	12.25
4854	OE1	GLU	A	318	56.621	21.580	49.603	1.00	13.30
4855	OE2	GLU	A	318	56.622	23.755	49.332	1.00	13.49
4856	C	GLU	A	318	51.675	22.343	48.560	1.00	10.76
4857	O	GLU	A	318	51.166	21.929	49.593	1.00	10.68
4858	N	LEU	A	319	51.638	21.667	47.417	1.00	10.71
4860	CA	LEU	A	319	51.057	20.335	47.337	1.00	10.55
4862	CB	LEU	A	319	50.876	19.909	45.878	1.00	10.67
4865	CG	LEU	A	319	49.841	20.737	45.110	1.00	10.56
4867	CD1	LEU	A	319	49.787	20.327	43.651	1.00	10.06
4871	CD2	LEU	A	319	48.466	20.608	45.753	1.00	10.35
4875	C	LEU	A	319	51.929	19.334	48.094	1.00	10.59
4876	O	LEU	A	319	53.151	19.331	47.967	1.00	10.10
4877	N	VAL	A	320	51.279	18.486	48.882	1.00	10.87
4879	CA	VAL	A	320	51.966	17.585	49.795	1.00	11.11
4881	CB	VAL	A	320	51.151	17.410	51.091	1.00	11.10
4883	CG1	VAL	A	320	51.809	16.394	52.028	1.00	11.37
4887	CG2	VAL	A	320	50.972	18.758	51.789	1.00	10.69
4891	C	VAL	A	320	52.178	16.236	49.117	1.00	11.41
4892	O	VAL	A	320	51.344	15.798	48.333	1.00	11.49
4893	N	ALA	A	321	53.305	15.592	49.407	1.00	11.87
4895	CA	ALA	A	321	53.580	14.237	48.930	1.00	12.19
4897	CB	ALA	A	321	54.849	13.685	49.596	1.00	12.50
4901	C	ALA	A	321	52.393	13.327	49.217	1.00	12.25
4902	O	ALA	A	321	51.933	13.241	50.354	1.00	12.30
4903	N	GLY	A	322	51.870	12.694	48.173	1.00	12.42
4905	CA	GLY	A	322	50.766	11.756	48.304	1.00	12.75
4908	C	GLY	A	322	49.367	12.357	48.244	1.00	12.86
4909	O	GLY	A	322	48.391	11.641	48.454	1.00	12.95
4910	N	TYR	A	323	49.256	13.647	47.931	1.00	13.17
4912	CA	TYR	A	323	47.957	14.332	47.904	1.00	13.58
4914	CB	TYR	A	323	48.117	15.836	47.607	1.00	13.42
4917	CG	TYR	A	323	48.302	16.159	46.141	1.00	13.11
4918	CD1	TYR	A	323	47.208	16.460	45.332	1.00	12.63
4920	CE1	TYR	A	323	47.367	16.742	43.983	1.00	12.13
4922	CZ	TYR	A	323	48.634	16.726	43.430	1.00	11.78
4923	OH	TYR	A	323	48.800	16.999	42.102	1.00	11.57
4925	CE2	TYR	A	323	49.738	16.430	44.211	1.00	12.43
4927	CD2	TYR	A	323	49.568	16.147	45.557	1.00	12.62
4929	C	TYR	A	323	46.987	13.707	46.901	1.00	13.96
4930	O	TYR	A	323	45.776	13.730	47.111	1.00	13.71
4931	N	GLN	A	324	47.522	13.150	45.818	1.00	14.65
4933	CA	GLN	A	324	46.696	12.572	44.757	1.00	15.33
4935	CB	GLN	A	324	47.553	12.220	43.533	1.00	15.41
4938	CG	GLN	A	324	48.089	13.449	42.807	1.00	15.91
4941	CD	GLN	A	324	49.054	13.117	41.681	1.00	16.94
4942	OE1	GLN	A	324	49.172	11.961	41.278	1.00	17.77
4943	NE2	GLN	A	324	49.751	14.131	41.175	1.00	16.22
4946	C	GLN	A	324	45.885	11.355	45.216	1.00	15.61
4947	O	GLN	A	324	44.905	10.996	44.566	1.00	15.76
4948	N	ASN	A	325	46.293	10.739	46.328	1.00	16.19

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4950	CA	ASN	A	325	45.571	9.615	46.934	1.00	16.67
4952	CB	ASN	A	325	46.559	8.674	47.635	1.00	16.92
4955	CG	ASN	A	325	47.581	8.099	46.683	1.00	18.10
4956	OD1	ASN	A	325	47.227	7.576	45.630	1.00	20.28
4957	ND2	ASN	A	325	48.860	8.199	47.043	1.00	19.45
4960	C	ASN	A	325	44.493	10.020	47.938	1.00	16.69
4961	O	ASN	A	325	43.843	9.153	48.520	1.00	17.30
4962	N	HIS	A	326	44.305	11.322	48.146	1.00	16.56
4964	CA	HIS	A	326	43.376	11.831	49.156	1.00	16.43
4966	CB	HIS	A	326	44.167	12.425	50.329	1.00	16.47
4969	CG	HIS	A	326	45.027	11.416	51.024	1.00	16.56
4970	ND1	HIS	A	326	44.500	10.357	51.731	1.00	16.47
4972	CE1	HIS	A	326	45.484	9.613	52.204	1.00	16.81
4974	NE2	HIS	A	326	46.630	10.150	51.824	1.00	16.63
4976	CD2	HIS	A	326	46.371	11.275	51.079	1.00	16.51
4978	C	HIS	A	326	42.374	12.837	48.579	1.00	16.15
4979	O	HIS	A	326	41.856	13.700	49.289	1.00	16.06
4980	N	LEU	A	327	42.098	12.702	47.285	1.00	15.84
4982	CA	LEU	A	327	41.060	13.478	46.620	1.00	15.79
4984	CB	LEU	A	327	41.540	13.922	45.235	1.00	15.93
4987	CG	LEU	A	327	42.870	14.688	45.239	1.00	15.85
4989	CD1	LEU	A	327	43.378	14.920	43.823	1.00	15.79
4993	CD2	LEU	A	327	42.715	16.003	45.979	1.00	16.33
4997	C	LEU	A	327	39.795	12.626	46.527	1.00	15.74
4998	O	LEU	A	327	39.796	11.457	46.927	1.00	15.54
4999	N	GLN	A	328	38.716	13.216	46.022	1.00	15.56
5001	CA	GLN	A	328	37.436	12.514	45.902	1.00	15.73
5003	CB	GLN	A	328	36.463	13.000	46.987	1.00	16.18
5006	CG	GLN	A	328	37.015	12.901	48.420	1.00	18.86
5009	CD	GLN	A	328	35.951	12.605	49.474	1.00	21.97
5010	OE1	GLN	A	328	36.269	12.511	50.658	1.00	25.17
5011	NE2	GLN	A	328	34.697	12.456	49.050	1.00	23.76
5014	C	GLN	A	328	36.815	12.698	44.517	1.00	14.70
5015	O	GLN	A	328	35.640	13.033	44.401	1.00	14.70
5016	N	LYS	A	329	37.605	12.464	43.470	1.00	13.86
5018	CA	LYS	A	329	37.144	12.676	42.099	1.00	13.08
5020	CB	LYS	A	329	38.252	12.377	41.083	1.00	12.96
5023	CG	LYS	A	329	37.872	12.727	39.643	1.00	12.63
5026	CD	LYS	A	329	39.080	12.714	38.717	1.00	12.37
5029	CE	LYS	A	329	38.741	13.292	37.356	1.00	12.53
5032	NZ	LYS	A	329	39.913	13.304	36.429	1.00	11.95
5036	C	LYS	A	329	35.895	11.870	41.746	1.00	12.64
5037	O	LYS	A	329	34.955	12.419	41.183	1.00	12.22
5038	N	GLU	A	330	35.884	10.578	42.065	1.00	12.20
5040	CA	GLU	A	330	34.758	9.723	41.685	1.00	12.11
5042	CB	GLU	A	330	35.009	8.249	42.020	1.00	12.12
5045	CG	GLU	A	330	33.962	7.331	41.390	1.00	12.23
5048	CD	GLU	A	330	34.160	5.858	41.695	1.00	12.23
5049	OE1	GLU	A	330	35.275	5.449	42.071	1.00	12.41
5050	OE2	GLU	A	330	33.182	5.106	41.546	1.00	12.10
5051	C	GLU	A	330	33.476	10.188	42.365	1.00	11.99
5052	O	GLU	A	330	32.433	10.280	41.731	1.00	11.67
5053	N	THR	A	331	33.571	10.471	43.658	1.00	11.91

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5055	CA	THR	A	331	32.446	10.987	44.435	1.00	12.09
5057	CB	THR	A	331	32.885	11.195	45.892	1.00	12.18
5059	OG1	THR	A	331	33.103	9.919	46.511	1.00	12.75
5061	CG2	THR	A	331	31.784	11.840	46.732	1.00	12.84
5065	C	THR	A	331	31.911	12.295	43.852	1.00	12.00
5066	O	THR	A	331	30.700	12.499	43.796	1.00	11.65
5067	N	HIS	A	332	32.817	13.169	43.412	1.00	11.95
5069	CA	HIS	A	332	32.439	14.480	42.893	1.00	11.91
5071	CB	HIS	A	332	33.659	15.406	42.820	1.00	11.96
5074	CG	HIS	A	332	34.186	15.812	44.161	1.00	12.02
5075	ND1	HIS	A	332	35.512	16.113	44.381	1.00	12.79
5077	CE1	HIS	A	332	35.684	16.431	45.653	1.00	13.18
5079	NE2	HIS	A	332	34.516	16.350	46.265	1.00	12.44
5081	CD2	HIS	A	332	33.563	15.962	45.354	1.00	12.47
5083	C	HIS	A	332	31.774	14.374	41.525	1.00	11.96
5084	O	HIS	A	332	30.790	15.057	41.259	1.00	11.84
5085	N	LEU	A	333	32.310	13.519	40.659	1.00	11.95
5087	CA	LEU	A	333	31.718	13.303	39.342	1.00	12.15
5089	CB	LEU	A	333	32.637	12.448	38.466	1.00	12.35
5092	CG	LEU	A	333	33.967	13.098	38.068	1.00	13.14
5094	CD1	LEU	A	333	34.859	12.082	37.367	1.00	14.23
5098	CD2	LEU	A	333	33.744	14.320	37.181	1.00	13.58
5102	C	LEU	A	333	30.346	12.647	39.486	1.00	12.02
5103	O	LEU	A	333	29.421	12.981	38.759	1.00	11.47
5104	N	ALA	A	334	30.227	11.729	40.441	1.00	11.95
5106	CA	ALA	A	334	28.955	11.080	40.751	1.00	12.28
5108	CB	ALA	A	334	29.153	10.009	41.810	1.00	12.24
5112	C	ALA	A	334	27.935	12.109	41.223	1.00	12.38
5113	O	ALA	A	334	26.781	12.079	40.816	1.00	12.29
5114	N	LEU	A	335	28.385	13.033	42.062	1.00	12.77
5116	CA	LEU	A	335	27.534	14.091	42.593	1.00	13.03
5118	CB	LEU	A	335	28.335	14.955	43.565	1.00	13.25
5121	CG	LEU	A	335	27.595	16.070	44.298	1.00	14.25
5123	CD1	LEU	A	335	26.607	15.492	45.290	1.00	15.18
5127	CD2	LEU	A	335	28.613	16.963	44.986	1.00	15.82
5131	C	LEU	A	335	26.957	14.956	41.474	1.00	12.87
5132	O	LEU	A	335	25.765	15.247	41.468	1.00	12.92
5133	N	LEU	A	336	27.804	15.350	40.528	1.00	12.77
5135	CA	LEU	A	336	27.387	16.205	39.416	1.00	12.81
5137	CB	LEU	A	336	28.611	16.822	38.728	1.00	12.79
5140	CG	LEU	A	336	29.490	17.731	39.592	1.00	13.01
5142	CD1	LEU	A	336	30.814	18.013	38.897	1.00	13.56
5146	CD2	LEU	A	336	28.776	19.034	39.940	1.00	13.15
5150	C	LEU	A	336	26.537	15.441	38.391	1.00	12.88
5151	O	LEU	A	336	25.557	15.973	37.880	1.00	12.68
5152	N	ASP	A	337	26.901	14.187	38.123	1.00	13.04
5154	CA	ASP	A	337	26.225	13.362	37.116	1.00	13.25
5156	CB	ASP	A	337	27.050	12.099	36.810	1.00	13.42
5159	CG	ASP	A	337	28.269	12.379	35.946	1.00	14.32
5160	OD1	ASP	A	337	28.263	13.374	35.194	1.00	16.21
5161	OD2	ASP	A	337	29.278	11.642	35.941	1.00	15.33
5162	C	ASP	A	337	24.821	12.926	37.532	1.00	13.22
5163	O	ASP	A	337	23.925	12.840	36.697	1.00	12.93

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5164	N	ASN	A	338	24.632	12.645	38.819	1.00	13.37
5166	CA	ASN	A	338	23.364	12.102	39.312	1.00	13.64
5168	CB	ASN	A	338	23.609	11.224	40.548	1.00	13.85
5171	CG	ASN	A	338	24.323	9.922	40.201	1.00	14.54
5172	OD1	ASN	A	338	25.233	9.487	40.910	1.00	16.43
5173	ND2	ASN	A	338	23.918	9.302	39.099	1.00	14.86
5176	C	ASN	A	338	22.298	13.169	39.589	1.00	13.50
5177	O	ASN	A	338	21.219	12.861	40.105	1.00	13.84
5178	N	ARG	A	339	22.584	14.413	39.212	1.00	13.19
5180	CA	ARG	A	339	21.616	15.491	39.348	1.00	12.90
5182	CB	ARG	A	339	22.294	16.855	39.205	1.00	12.58
5185	CG	ARG	A	339	23.347	17.141	40.272	1.00	12.17
5188	CD	ARG	A	339	24.052	18.483	40.111	1.00	11.56
5191	NE	ARG	A	339	24.788	18.577	38.847	1.00	10.52
5193	CZ	ARG	A	339	25.338	19.688	38.371	1.00	10.16
5194	NH1	ARG	A	339	25.246	20.831	39.037	1.00	9.64
5197	NH2	ARG	A	339	25.978	19.655	37.210	1.00	10.28
5200	C	ARG	A	339	20.513	15.357	38.306	1.00	13.10
5201	O	ARG	A	339	20.714	14.764	37.246	1.00	12.95
5202	N	THR	A	340	19.356	15.925	38.633	1.00	13.21
5204	CA	THR	A	340	18.201	15.974	37.753	1.00	13.55
5206	CB	THR	A	340	16.915	15.816	38.585	1.00	13.57
5208	OG1	THR	A	340	16.940	14.564	39.281	1.00	13.66
5210	CG2	THR	A	340	15.671	15.733	37.691	1.00	14.07
5214	C	THR	A	340	18.173	17.311	37.023	1.00	13.84
5215	O	THR	A	340	18.227	18.371	37.654	1.00	13.89
5216	N	GLU	A	341	18.084	17.260	35.697	1.00	14.08
5218	CA	GLU	A	341	17.932	18.460	34.891	1.00	14.42
5220	CB	GLU	A	341	18.218	18.172	33.419	1.00	14.68
5223	CG	GLU	A	341	18.241	19.431	32.562	1.00	15.06
5226	CD	GLU	A	341	18.585	19.167	31.110	1.00	16.30
5227	OE1	GLU	A	341	18.652	20.149	30.345	1.00	18.47
5228	OE2	GLU	A	341	18.784	17.994	30.730	1.00	17.71
5229	C	GLU	A	341	16.520	19.018	35.018	1.00	14.64
5230	O	GLU	A	341	15.540	18.284	34.878	1.00	14.46
5231	N	LEU	A	342	16.435	20.325	35.257	1.00	14.72
5233	CA	LEU	A	342	15.169	21.037	35.315	1.00	14.92
5235	CB	LEU	A	342	15.204	22.113	36.409	1.00	15.14
5238	CG	LEU	A	342	15.439	21.660	37.854	1.00	15.76
5240	CD1	LEU	A	342	15.562	22.870	38.763	1.00	16.15
5244	CD2	LEU	A	342	14.333	20.734	38.340	1.00	16.53
5248	C	LEU	A	342	14.897	21.716	33.978	1.00	14.85
5249	O	LEU	A	342	15.806	22.250	33.349	1.00	14.61
5250	N	SER	A	343	13.636	21.694	33.552	1.00	14.71
5252	CA	SER	A	343	13.176	22.534	32.458	1.00	14.55
5254	CB	SER	A	343	11.771	22.112	32.027	1.00	14.63
5257	OG	SER	A	343	10.819	22.501	33.002	1.00	13.80
5259	C	SER	A	343	13.146	23.970	32.961	1.00	14.64
5260	O	SER	A	343	13.220	24.196	34.162	1.00	14.05
5261	N	ILE	A	344	13.026	24.936	32.053	1.00	14.98
5263	CA	ILE	A	344	12.940	26.343	32.447	1.00	15.27
5265	CB	ILE	A	344	12.850	27.295	31.210	1.00	15.60
5267	CG1	ILE	A	344	12.845	28.764	31.650	1.00	15.91

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5270	CD1	ILE	A	344	14.197	29.297	32.043	1.00	16.15
5274	CG2	ILE	A	344	11.597	27.020	30.363	1.00	16.26
5278	C	ILE	A	344	11.766	26.567	33.398	1.00	15.22
5279	O	ILE	A	344	11.903	27.281	34.392	1.00	15.26
5280	N	ALA	A	345	10.626	25.948	33.108	1.00	14.85
5282	CA	ALA	A	345	9.433	26.132	33.932	1.00	14.73
5284	CB	ALA	A	345	8.218	25.497	33.262	1.00	14.93
5288	C	ALA	A	345	9.636	25.558	35.338	1.00	14.48
5289	O	ALA	A	345	9.194	26.148	36.323	1.00	14.31
5290	N	GLU	A	346	10.307	24.413	35.422	1.00	14.15
5292	CA	GLU	A	346	10.624	23.786	36.707	1.00	14.02
5294	CB	GLU	A	346	11.146	22.363	36.496	1.00	13.95
5297	CG	GLU	A	346	10.062	21.362	36.117	1.00	14.71
5300	CD	GLU	A	346	10.605	20.037	35.605	1.00	15.06
5301	OE1	GLU	A	346	9.819	19.069	35.512	1.00	16.85
5302	OE2	GLU	A	346	11.806	19.950	35.289	1.00	13.70
5303	C	GLU	A	346	11.642	24.615	37.504	1.00	13.65
5304	O	GLU	A	346	11.509	24.767	38.715	1.00	13.64
5305	N	TYR	A	347	12.646	25.149	36.816	1.00	13.27
5307	CA	TYR	A	347	13.638	26.042	37.426	1.00	13.05
5309	CB	TYR	A	347	14.718	26.426	36.403	1.00	12.89
5312	CG	TYR	A	347	15.455	27.726	36.686	1.00	13.10
5313	CD1	TYR	A	347	15.277	28.843	35.871	1.00	13.64
5315	CE1	TYR	A	347	15.958	30.036	36.120	1.00	13.73
5317	CZ	TYR	A	347	16.827	30.119	37.191	1.00	13.43
5318	OH	TYR	A	347	17.505	31.297	37.437	1.00	13.87
5320	CE2	TYR	A	347	17.021	29.025	38.011	1.00	13.24
5322	CD2	TYR	A	347	16.338	27.834	37.754	1.00	12.87
5324	C	TYR	A	347	12.976	27.294	37.999	1.00	13.02
5325	O	TYR	A	347	13.245	27.673	39.134	1.00	12.68
5326	N	GLU	A	348	12.097	27.919	37.219	1.00	13.09
5328	CA	GLU	A	348	11.475	29.176	37.623	1.00	13.46
5330	CB	GLU	A	348	10.756	29.839	36.436	1.00	13.51
5333	CG	GLU	A	348	11.722	30.349	35.368	1.00	14.34
5336	CD	GLU	A	348	11.114	31.371	34.418	1.00	15.48
5337	OE1	GLU	A	348	9.910	31.274	34.106	1.00	16.56
5338	OE2	GLU	A	348	11.853	32.272	33.974	1.00	15.67
5339	C	GLU	A	348	10.534	28.981	38.815	1.00	13.52
5340	O	GLU	A	348	10.436	29.855	39.670	1.00	13.44
5341	N	ALA	A	349	9.863	27.833	38.880	1.00	13.86
5343	CA	ALA	A	349	8.988	27.520	40.012	1.00	14.18
5345	CB	ALA	A	349	8.127	26.300	39.707	1.00	14.18
5349	C	ALA	A	349	9.814	27.294	41.282	1.00	14.24
5350	O	ALA	A	349	9.505	27.849	42.341	1.00	14.45
5351	N	MSE	A	350	10.871	26.494	41.166	1.00	14.32
5353	CA	MSE	A	350	11.759	26.214	42.295	1.00	14.50
5355	CB	MSE	A	350	12.809	25.168	41.906	1.00	14.42
5358	CG	MSE	A	350	13.668	24.690	43.076	1.00	14.25
5361	SE	MSE	A	350	14.904	23.272	42.580	1.00	14.19
5362	CE	MSE	A	350	13.645	21.797	42.383	1.00	14.41
5366	C	MSE	A	350	12.454	27.486	42.790	1.00	14.59
5367	O	MSE	A	350	12.580	27.708	43.991	1.00	14.60
5368	N	PHE	A	351	12.883	28.323	41.856	1.00	14.91

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5370	CA	PHE	A	351	13.594	29.555	42.182	1.00	15.21
5372	CB	PHE	A	351	14.116	30.215	40.896	1.00	15.04
5375	CG	PHE	A	351	14.958	31.436	41.137	1.00	14.10
5376	CD1	PHE	A	351	14.368	32.661	41.423	1.00	13.66
5378	CE1	PHE	A	351	15.141	33.782	41.648	1.00	13.50
5380	CZ	PHE	A	351	16.523	33.694	41.579	1.00	13.30
5382	CE2	PHE	A	351	17.120	32.486	41.293	1.00	13.49
5384	CD2	PHE	A	351	16.342	31.363	41.071	1.00	13.51
5386	C	PHE	A	351	12.694	30.533	42.930	1.00	15.78
5387	O	PHE	A	351	13.110	31.138	43.918	1.00	16.13
5388	N	ALA	A	352	11.462	30.678	42.454	1.00	16.47
5390	CA	ALA	A	352	10.562	31.729	42.929	1.00	17.03
5392	CB	ALA	A	352	9.472	31.993	41.896	1.00	17.21
5396	C	ALA	A	352	9.934	31.404	44.286	1.00	17.53
5397	O	ALA	A	352	9.524	32.308	45.012	1.00	17.43
5398	N	GLU	A	353	9.878	30.118	44.629	1.00	18.01
5400	CA	GLU	A	353	9.221	29.681	45.857	1.00	18.57
5402	CB	GLU	A	353	9.292	28.157	46.004	1.00	18.73
5405	CG	GLU	A	353	8.269	27.580	46.974	1.00	19.70
5408	CD	GLU	A	353	8.309	26.062	47.054	1.00	20.97
5409	OE1	GLU	A	353	7.481	25.492	47.795	1.00	23.03
5410	OE2	GLU	A	353	9.171	25.433	46.395	1.00	20.91
5411	C	GLU	A	353	9.834	30.364	47.076	1.00	18.59
5412	O	GLU	A	353	11.056	30.440	47.218	1.00	18.77
5413	N	THR	A	354	8.969	30.889	47.934	1.00	18.65
5415	CA	THR	A	354	9.393	31.526	49.171	1.00	18.59
5417	CB	ATHR	A	354	8.729	32.908	49.340	0.65	18.54
5419	OG1	ATHR	A	354	7.318	32.807	49.117	0.65	18.59
5421	CG2	ATHR	A	354	9.206	33.874	48.270	0.65	18.76
5425	C	THR	A	354	9.030	30.631	50.340	1.00	18.54
5426	O	THR	A	354	8.105	29.817	50.259	1.00	18.83
5427	N	LEU	A	355	9.795	30.768	51.413	1.00	18.42
5429	CA	LEU	A	355	9.529	30.068	52.655	1.00	18.38
5431	CB	LEU	A	355	10.738	29.231	53.072	1.00	18.30
5434	CG	LEU	A	355	10.609	28.468	54.396	1.00	18.64
5436	CD1	LEU	A	355	9.409	27.526	54.379	1.00	18.61
5440	CD2	LEU	A	355	11.888	27.707	54.680	1.00	18.77
5444	C	LEU	A	355	9.231	31.123	53.705	1.00	17.93
5445	O	LEU	A	355	10.080	31.958	54.002	1.00	17.93
5446	N	ASP	A	356	8.007	31.099	54.221	1.00	17.67
5448	CA	ASP	A	356	7.603	31.937	55.342	1.00	17.33
5450	CB	ASP	A	356	6.134	32.339	55.197	1.00	17.51
5453	CG	ASP	A	356	5.705	33.391	56.207	1.00	17.64
5454	OD1	ASP	A	356	6.474	33.697	57.144	1.00	17.26
5455	OD2	ASP	A	356	4.604	33.967	56.136	1.00	18.45
5456	C	ASP	A	356	7.823	31.150	56.636	1.00	16.92
5457	O	ASP	A	356	7.016	30.296	56.996	1.00	16.46
5458	N	THR	A	357	8.921	31.453	57.325	1.00	16.68
5460	CA	THR	A	357	9.314	30.732	58.539	1.00	16.73
5462	CB	THR	A	357	10.809	30.971	58.868	1.00	16.81
5464	OG1	THR	A	357	11.066	32.372	58.977	1.00	17.70
5466	CG2	THR	A	357	11.719	30.510	57.725	1.00	17.29
5470	C	THR	A	357	8.462	31.079	59.763	1.00	16.35

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5471	O	THR	A	357	8.589	30.435	60.802	1.00	16.08
5472	N	ASP	A	358	7.611	32.096	59.646	1.00	16.13
5474	CA	ASP	A	358	6.614	32.398	60.676	1.00	16.27
5476	CB	ASP	A	358	6.080	33.824	60.512	1.00	16.34
5479	CG	ASP	A	358	7.090	34.877	60.915	1.00	16.62
5480	OD1	ASP	A	358	8.037	34.558	61.666	1.00	17.57
5481	OD2	ASP	A	358	7.004	36.058	60.537	1.00	17.02
5482	C	ASP	A	358	5.437	31.421	60.662	1.00	16.16
5483	O	ASP	A	358	4.621	31.431	61.580	1.00	16.17
5484	N	ILE	A	359	5.351	30.595	59.620	1.00	16.11
5486	CA	ILE	A	359	4.297	29.593	59.489	1.00	16.26
5488	CB	ILE	A	359	3.732	29.572	58.045	1.00	16.55
5490	CG1	ILE	A	359	3.285	30.971	57.601	1.00	17.22
5493	CD1	ILE	A	359	2.109	31.539	58.375	1.00	18.42
5497	CG2	ILE	A	359	2.574	28.561	57.929	1.00	16.87
5501	C	ILE	A	359	4.847	28.219	59.830	1.00	15.89
5502	O	ILE	A	359	5.779	27.742	59.187	1.00	15.72
5503	N	ASP	A	360	4.267	27.589	60.845	1.00	15.65
5505	CA	ASP	A	360	4.597	26.214	61.190	1.00	15.51
5507	CB	ASP	A	360	3.920	25.800	62.498	1.00	15.42
5510	CG	ASP	A	360	4.374	26.640	63.673	1.00	15.22
5511	OD1	ASP	A	360	3.644	26.709	64.677	1.00	14.30
5512	OD2	ASP	A	360	5.446	27.281	63.671	1.00	14.41
5513	C	ASP	A	360	4.179	25.294	60.054	1.00	15.39
5514	O	ASP	A	360	3.063	25.380	59.554	1.00	15.44
5515	N	GLN	A	361	5.098	24.429	59.643	1.00	15.26
5517	CA	GLN	A	361	4.896	23.568	58.484	1.00	15.11
5519	CB	GLN	A	361	4.911	24.400	57.196	1.00	15.34
5522	CG	GLN	A	361	6.217	25.165	56.961	1.00	15.68
5525	CD	GLN	A	361	6.119	26.161	55.817	1.00	16.76
5526	OE1	GLN	A	361	5.988	25.768	54.661	1.00	16.89
5527	NE2	GLN	A	361	6.190	27.449	56.136	1.00	17.13
5530	C	GLN	A	361	5.975	22.500	58.393	1.00	14.90
5531	O	GLN	A	361	7.018	22.587	59.037	1.00	14.23
5532	N	THR	A	362	5.716	21.506	57.557	1.00	14.83
5534	CA	THR	A	362	6.671	20.453	57.262	1.00	15.17
5536	CB	THR	A	362	6.036	19.085	57.557	1.00	15.31
5538	OG1	THR	A	362	5.428	19.100	58.860	1.00	15.89
5540	CG2	THR	A	362	7.099	18.001	57.648	1.00	15.70
5544	C	THR	A	362	7.045	20.540	55.789	1.00	15.03
5545	O	THR	A	362	6.169	20.636	54.934	1.00	15.06
5546	N	LEU	A	363	8.342	20.518	55.500	1.00	14.98
5548	CA	LEU	A	363	8.831	20.495	54.126	1.00	15.07
5550	CB	BLEU	A	363	10.037	21.426	53.950	0.35	15.14
5551	CB	ALEU	A	363	10.030	21.433	53.957	0.65	15.12
5556	CG	BLEU	A	363	9.823	22.946	54.005	0.35	15.70
5557	CG	ALEU	A	363	9.744	22.938	53.973	0.65	15.75
5560	CD1	BLEU	A	363	8.571	23.374	53.246	0.35	15.88
5561	CD1	ALEU	A	363	9.140	23.378	55.299	0.65	16.69
5568	CD2	BLEU	A	363	9.770	23.444	55.442	0.35	16.27
5569	CD2	ALEU	A	363	11.016	23.720	53.674	0.65	15.48
5576	C	LEU	A	363	9.235	19.064	53.819	1.00	14.86
5577	O	LEU	A	363	9.811	18.394	54.675	1.00	14.87

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5578	N	GLU	A	364	8.921	18.600	52.612	1.00	14.49
5580	CA	GLU	A	364	9.267	17.250	52.170	1.00	14.45
5582	CB	GLU	A	364	8.042	16.537	51.573	1.00	14.64
5585	CG	GLU	A	364	8.334	15.346	50.655	1.00	15.61
5588	CD	GLU	A	364	9.295	14.309	51.232	1.00	17.24
5589	OE1	GLU	A	364	9.482	14.229	52.475	1.00	17.33
5590	OE2	GLU	A	364	9.871	13.551	50.422	1.00	17.72
5591	C	GLU	A	364	10.405	17.321	51.162	1.00	13.90
5592	O	GLU	A	364	10.347	18.067	50.187	1.00	13.79
5593	N	ASP	A	365	11.441	16.535	51.419	1.00	13.54
5595	CA	ASP	A	365	12.632	16.501	50.581	1.00	13.42
5597	CB	ASP	A	365	13.518	17.715	50.893	1.00	13.35
5600	CG	ASP	A	365	14.550	17.999	49.807	1.00	13.84
5601	OD1	ASP	A	365	15.117	17.045	49.239	1.00	13.44
5602	OD2	ASP	A	365	14.863	19.157	49.461	1.00	13.26
5603	C	ASP	A	365	13.367	15.187	50.849	1.00	13.21
5604	O	ASP	A	365	13.516	14.779	52.001	1.00	12.99
5605	N	GLU	A	366	13.816	14.526	49.784	1.00	13.11
5607	CA	GLU	A	366	14.494	13.233	49.887	1.00	13.06
5609	CB	GLU	A	366	14.522	12.539	48.514	1.00	13.38
5612	CG	AGLU	A	366	13.154	12.149	47.966	0.65	13.53
5615	CD	AGLU	A	366	13.237	11.143	46.825	0.65	14.22
5616	OE1AGLU	A	366		12.245	10.417	46.599	0.65	14.91
5617	OE2AGLU	A	366		14.292	11.064	46.158	0.65	14.08
5618	C	GLU	A	366	15.929	13.353	50.403	1.00	12.99
5619	O	GLU	A	366	16.506	12.372	50.870	1.00	12.92
5620	N	LEU	A	367	16.509	14.547	50.310	1.00	12.76
5622	CA	LEU	A	367	17.924	14.741	50.618	1.00	12.46
5624	CB	LEU	A	367	18.417	16.074	50.041	1.00	12.48
5627	CG	LEU	A	367	19.920	16.360	50.154	1.00	12.94
5629	CD1	LEU	A	367	20.740	15.404	49.296	1.00	14.22
5633	CD2	LEU	A	367	20.221	17.801	49.781	1.00	12.50
5637	C	LEU	A	367	18.202	14.702	52.116	1.00	12.25
5638	O	LEU	A	367	17.457	15.271	52.917	1.00	12.00
5639	N	LYS	A	368	19.289	14.031	52.479	1.00	11.83
5641	CA	LYS	A	368	19.790	14.040	53.845	1.00	11.73
5643	CB	LYS	A	368	21.010	13.120	53.972	1.00	11.82
5646	CG	LYS	A	368	21.418	12.780	55.403	1.00	12.46
5649	CD	LYS	A	368	22.741	12.019	55.413	1.00	13.39
5652	CE	LYS	A	368	22.925	11.207	56.682	1.00	14.11
5655	NZ	LYS	A	368	24.215	10.465	56.682	1.00	14.32
5659	C	LYS	A	368	20.152	15.478	54.240	1.00	11.19
5660	O	LYS	A	368	20.703	16.239	53.439	1.00	10.84
5661	N	TYR	A	369	19.798	15.834	55.471	1.00	10.91
5663	CA	TYR	A	369	20.042	17.157	56.049	1.00	10.67
5665	CB	TYR	A	369	21.541	17.486	56.060	1.00	10.69
5668	CG	TYR	A	369	22.389	16.472	56.798	1.00	11.38
5669	CD1	TYR	A	369	23.471	15.859	56.177	1.00	12.19
5671	CE1	TYR	A	369	24.256	14.930	56.852	1.00	13.08
5673	CZ	TYR	A	369	23.958	14.604	58.165	1.00	13.09
5674	OH	TYR	A	369	24.733	13.690	58.829	1.00	14.74
5676	CE2	TYR	A	369	22.889	15.196	58.808	1.00	13.03
5678	CD2	TYR	A	369	22.110	16.128	58.123	1.00	12.38

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5680	C	TYR	A	369	19.239	18.297	55.407	1.00	10.49
5681	O	TYR	A	369	19.521	19.472	55.667	1.00	10.34
5682	N	SER	A	370	18.235	17.958	54.597	1.00	9.93
5684	CA	SER	A	370	17.258	18.939	54.136	1.00	10.02
5686	CB	SER	A	370	16.434	18.395	52.963	1.00	9.93
5689	OG	SER	A	370	15.825	17.156	53.296	1.00	10.17
5691	C	SER	A	370	16.327	19.320	55.286	1.00	9.92
5692	O	SER	A	370	16.237	18.612	56.286	1.00	9.97
5693	N	ILE	A	371	15.627	20.436	55.136	1.00	10.13
5695	CA	ILE	A	371	14.715	20.913	56.165	1.00	10.20
5697	CB	ILE	A	371	14.286	22.372	55.894	1.00	10.24
5699	CG1	ILE	A	371	15.496	23.311	55.868	1.00	10.27
5702	CD1	ILE	A	371	15.233	24.609	55.107	1.00	10.40
5706	CG2	ILE	A	371	13.297	22.848	56.964	1.00	9.83
5710	C	ILE	A	371	13.476	20.022	56.212	1.00	10.36
5711	O	ILE	A	371	12.886	19.721	55.169	1.00	10.09
5712	N	SER	A	372	13.107	19.600	57.422	1.00	10.60
5714	CA	SER	A	372	11.821	18.963	57.688	1.00	11.05
5716	CB	SER	A	372	11.994	17.690	58.529	1.00	11.11
5719	OG	SER	A	372	12.698	17.956	59.726	1.00	9.90
5721	C	SER	A	372	10.894	19.972	58.381	1.00	11.52
5722	O	SER	A	372	10.160	20.678	57.716	1.00	12.46
5723	N	ALA	A	373	10.946	20.081	59.704	1.00	11.97
5725	CA	ALA	A	373	10.030	20.968	60.421	1.00	11.70
5727	CB	ALA	A	373	9.876	20.505	61.859	1.00	11.92
5731	C	ALA	A	373	10.481	22.431	60.395	1.00	11.76
5732	O	ALA	A	373	11.673	22.721	60.404	1.00	11.09
5733	N	ILE	A	374	9.507	23.335	60.311	1.00	11.77
5735	CA	ILE	A	374	9.649	24.710	60.782	1.00	12.11
5737	CB	ILE	A	374	9.333	25.751	59.687	1.00	12.41
5739	CG1	ILE	A	374	10.153	25.492	58.420	1.00	13.61
5742	CD1	ILE	A	374	11.641	25.634	58.607	1.00	14.48
5746	CG2	ILE	A	374	9.597	27.167	60.214	1.00	12.27
5750	C	ILE	A	374	8.649	24.841	61.922	1.00	11.96
5751	O	ILE	A	374	7.449	24.635	61.727	1.00	11.50
5752	N	ASN	A	375	9.145	25.157	63.112	1.00	11.72
5754	CA	ASN	A	375	8.316	25.217	64.304	1.00	11.69
5756	CB	ASN	A	375	8.426	23.907	65.098	1.00	11.66
5759	CG	ASN	A	375	7.452	23.845	66.274	1.00	12.59
5760	OD1	ASN	A	375	7.663	23.104	67.233	1.00	14.92
5761	ND2	ASN	A	375	6.380	24.614	66.195	1.00	13.50
5764	C	ASN	A	375	8.753	26.388	65.166	1.00	11.38
5765	O	ASN	A	375	9.876	26.406	65.669	1.00	11.16
5766	N	ASN	A	376	7.859	27.352	65.345	1.00	11.20
5768	CA	ASN	A	376	8.185	28.592	66.037	1.00	11.21
5770	CB	ASN	A	376	8.319	28.332	67.543	1.00	11.11
5773	CG	ASN	A	376	8.185	29.597	68.373	1.00	11.35
5774	OD1	ASN	A	376	7.387	30.484	68.058	1.00	10.26
5775	ND2	ASN	A	376	8.971	29.686	69.441	1.00	11.55
5778	C	ASN	A	376	9.455	29.232	65.453	1.00	11.05
5779	O	ASN	A	376	10.330	29.684	66.189	1.00	10.77
5780	N	THR	A	377	9.524	29.246	64.117	1.00	10.89
5782	CA	THR	A	377	10.668	29.735	63.318	1.00	10.98

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5784	CB	THR	A	377	11.077	31.200	63.674	1.00	10.89
5786	OG1	THR	A	377	11.735	31.236	64.946	1.00	10.33
5788	CG2	THR	A	377	9.859	32.111	63.832	1.00	11.01
5792	C	THR	A	377	11.916	28.840	63.316	1.00	10.94
5793	O	THR	A	377	12.841	29.086	62.543	1.00	10.97
5794	N	VAL	A	378	11.944	27.807	64.153	1.00	11.19
5796	CA	VAL	A	378	13.105	26.927	64.250	1.00	11.25
5798	CB	VAL	A	378	13.203	26.264	65.640	1.00	11.31
5800	CG1	VAL	A	378	14.437	25.358	65.726	1.00	11.42
5804	CG2	VAL	A	378	13.226	27.323	66.735	1.00	11.87
5808	C	VAL	A	378	13.066	25.834	63.188	1.00	11.32
5809	O	VAL	A	378	12.068	25.126	63.043	1.00	11.24
5810	N	ARG	A	379	14.174	25.685	62.468	1.00	11.42
5812	CA	ARG	A	379	14.314	24.646	61.462	1.00	11.70
5814	CB	ARG	A	379	15.297	25.081	60.372	1.00	11.87
5817	CG	ARG	A	379	14.855	26.293	59.564	1.00	12.48
5820	CD	ARG	A	379	15.988	26.961	58.799	1.00	13.13
5823	NE	ARG	A	379	15.572	28.253	58.248	1.00	13.12
5825	CZ	ARG	A	379	15.731	28.646	56.983	1.00	12.53
5826	NH1	ARG	A	379	16.342	27.885	56.084	1.00	12.53
5829	NH2	ARG	A	379	15.290	29.844	56.618	1.00	12.90
5832	C	ARG	A	379	14.822	23.358	62.104	1.00	11.69
5833	O	ARG	A	379	15.712	23.385	62.960	1.00	11.39
5834	N	SER	A	380	14.239	22.238	61.692	1.00	11.60
5836	CA	SER	A	380	14.797	20.927	61.955	1.00	11.82
5838	CB	SER	A	380	13.747	20.015	62.581	1.00	11.99
5841	OG	SER	A	380	13.304	20.542	63.814	1.00	12.10
5843	C	SER	A	380	15.284	20.347	60.635	1.00	11.85
5844	O	SER	A	380	14.803	20.730	59.572	1.00	11.84
5845	N	TYR	A	381	16.244	19.435	60.720	1.00	11.95
5847	CA	TYR	A	381	16.850	18.797	59.557	1.00	12.18
5849	CB	TYR	A	381	18.313	19.235	59.429	1.00	12.11
5852	CG	TYR	A	381	18.447	20.729	59.282	1.00	10.28
5853	CD1	TYR	A	381	18.402	21.325	58.033	1.00	9.25
5855	CE1	TYR	A	381	18.498	22.699	57.886	1.00	8.92
5857	CZ	TYR	A	381	18.630	23.497	59.005	1.00	8.09
5858	OH	TYR	A	381	18.718	24.852	58.854	1.00	7.57
5860	CE2	TYR	A	381	18.668	22.934	60.265	1.00	8.75
5862	CD2	TYR	A	381	18.570	21.549	60.398	1.00	9.56
5864	C	TYR	A	381	16.755	17.278	59.688	1.00	12.78
5865	O	TYR	A	381	17.047	16.718	60.748	1.00	12.72
5866	N	ARG	A	382	16.328	16.611	58.621	1.00	13.67
5868	CA	ARG	A	382	16.218	15.152	58.648	1.00	14.36
5870	CB	ARG	A	382	15.333	14.605	57.507	1.00	14.27
5873	CG	ARG	A	382	15.536	15.214	56.133	1.00	13.64
5876	CD	ARG	A	382	14.693	14.563	55.036	1.00	13.08
5879	NE	ARG	A	382	13.254	14.715	55.266	1.00	11.85
5881	CZ	ARG	A	382	12.553	15.828	55.060	1.00	11.18
5882	NH1	ARG	A	382	11.252	15.838	55.316	1.00	11.19
5885	NH2	ARG	A	382	13.127	16.931	54.600	1.00	10.55
5888	C	ARG	A	382	17.614	14.519	58.667	1.00	15.14
5889	O	ARG	A	382	18.498	14.918	57.914	1.00	15.32
5890	N	ASN	A	383	17.803	13.555	59.564	1.00	16.08

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5892	CA	ASN	A	383	19.102	12.918	59.794	1.00	16.97
5894	CB	AASN	A	383	19.156	12.301	61.202	0.65	16.85
5897	CG	AASN	A	383	19.078	13.343	62.307	0.65	17.39
5898	OD1AASN	A	383		18.410	13.138	63.322	0.65	18.43
5899	ND2AASN	A	383		19.767	14.461	62.120	0.65	17.07
5902	C	ASN	A	383	19.428	11.837	58.769	1.00	17.67
5903	O	ASN	A	383	20.563	11.355	58.711	1.00	17.96
5904	N	ALA	A	384	18.430	11.440	57.985	1.00	18.47
5906	CA	ALA	A	384	18.634	10.473	56.909	1.00	18.93
5908	CB	ALA	A	384	18.130	9.090	57.336	1.00	19.18
5912	C	ALA	A	384	17.924	10.921	55.642	1.00	19.23
5913	O	ALA	A	384	16.879	11.566	55.699	1.00	19.29
5914	N	GLY	A	385	18.501	10.582	54.496	1.00	19.64
5916	CA	GLY	A	385	17.799	10.700	53.233	1.00	20.00
5919	C	GLY	A	385	16.771	9.587	53.115	1.00	20.41
5920	O	GLY	A	385	16.734	8.670	53.939	1.00	20.69
5921	N	HIS	A	386	15.926	9.674	52.096	1.00	20.83
5923	CA	HIS	A	386	14.971	8.611	51.796	1.00	21.17
5925	CB	HIS	A	386	13.735	8.715	52.705	1.00	21.06
5928	CG	HIS	A	386	12.963	9.992	52.544	1.00	20.61
5929	ND1	HIS	A	386	13.073	11.045	53.427	1.00	20.63
5931	CE1	HIS	A	386	12.276	12.027	53.044	1.00	19.49
5933	NE2	HIS	A	386	11.650	11.647	51.945	1.00	19.98
5935	CD2	HIS	A	386	12.058	10.377	51.613	1.00	20.28
5937	C	HIS	A	386	14.553	8.620	50.328	1.00	21.64
5938	O	HIS	A	386	14.799	9.583	49.602	1.00	21.80
5939	N	ALA	A	387	13.948	7.518	49.902	1.00	22.16
5941	CA	ALA	A	387	13.315	7.411	48.591	1.00	22.56
5943	CB	ALA	A	387	14.329	6.994	47.540	1.00	22.65
5947	C	ALA	A	387	12.204	6.373	48.725	1.00	22.96
5948	O	ALA	A	387	12.481	5.174	48.824	1.00	23.38
5949	N	ALA	A	388	10.954	6.839	48.744	1.00	23.23
5951	CA	ALA	A	388	9.829	6.021	49.210	1.00	23.31
5953	CB	ALA	A	388	8.609	6.911	49.495	1.00	23.34
5957	C	ALA	A	388	9.449	4.890	48.249	1.00	23.62
5958	O	ALA	A	388	9.783	4.930	47.058	1.00	24.07
5959	N	THR	B	2	54.358	38.490	75.937	1.00	11.97
5961	CA	THR	B	2	52.902	38.329	76.203	1.00	12.11
5963	CB	THR	B	2	52.503	39.021	77.518	1.00	12.22
5965	OG1	THR	B	2	52.909	40.395	77.491	1.00	12.34
5967	CG2	THR	B	2	53.253	38.421	78.709	1.00	13.31
5971	C	THR	B	2	52.089	38.913	75.061	1.00	11.80
5972	O	THR	B	2	52.613	39.663	74.238	1.00	11.83
5975	N	ILE	B	3	50.813	38.539	75.013	1.00	11.52
5977	CA	ILE	B	3	49.856	39.041	74.022	1.00	11.38
5979	CB	ILE	B	3	49.672	38.032	72.868	1.00	11.66
5981	CG1	ILE	B	3	51.000	37.716	72.174	1.00	12.99
5984	CD1	ILE	B	3	51.015	36.354	71.556	1.00	14.40
5988	CG2	ILE	B	3	48.670	38.565	71.844	1.00	12.11
5992	C	ILE	B	3	48.506	39.234	74.689	1.00	10.74
5993	O	ILE	B	3	48.089	38.401	75.489	1.00	10.37
5994	N	GLY	B	4	47.807	40.310	74.343	1.00	10.22
5996	CA	GLY	B	4	46.466	40.515	74.859	1.00	10.00

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5999	C	GLY	B	4	45.862	41.875	74.579	1.00	9.71
6000	O	GLY	B	4	46.128	42.486	73.544	1.00	9.39
6001	N	ILE	B	5	45.017	42.324	75.503	1.00	9.42
6003	CA	ILE	B	5	44.315	43.589	75.373	1.00	9.31
6005	CB	ILE	B	5	43.039	43.603	76.249	1.00	9.46
6007	CG1	ILE	B	5	42.068	42.504	75.785	1.00	9.81
6010	CD1	ILE	B	5	40.958	42.173	76.784	1.00	10.10
6014	CG2	ILE	B	5	42.354	44.963	76.167	1.00	9.61
6018	C	ILE	B	5	45.261	44.730	75.735	1.00	9.06
6019	O	ILE	B	5	45.571	44.958	76.901	1.00	8.73
6020	N	ASP	B	6	45.739	45.416	74.707	1.00	8.88
6022	CA	ASP	B	6	46.635	46.551	74.866	1.00	8.82
6024	CB	ASP	B	6	47.421	46.772	73.574	1.00	8.72
6027	CG	ASP	B	6	48.464	47.851	73.709	1.00	9.13
6028	OD1	ASP	B	6	48.569	48.693	72.792	1.00	10.02
6029	OD2	ASP	B	6	49.217	47.938	74.699	1.00	8.01
6030	C	ASP	B	6	45.856	47.817	75.230	1.00	8.64
6031	O	ASP	B	6	46.280	48.594	76.082	1.00	8.63
6032	N	LYS	B	7	44.730	48.022	74.555	1.00	8.52
6034	CA	LYS	B	7	43.843	49.150	74.828	1.00	8.56
6036	CB	LYS	B	7	44.014	50.252	73.779	1.00	8.57
6039	CG	LYS	B	7	45.424	50.767	73.601	1.00	8.68
6042	CD	LYS	B	7	45.459	51.789	72.481	1.00	8.18
6045	CE	LYS	B	7	46.854	52.317	72.231	1.00	7.72
6048	NZ	LYS	B	7	46.811	53.444	71.253	1.00	7.10
6052	C	LYS	B	7	42.400	48.688	74.806	1.00	8.49
6053	O	LYS	B	7	42.063	47.709	74.144	1.00	8.34
6054	N	ILE	B	8	41.550	49.400	75.533	1.00	8.42
6056	CA	ILE	B	8	40.128	49.108	75.568	1.00	8.31
6058	CB	ILE	B	8	39.829	47.934	76.536	1.00	8.48
6060	CG1	ILE	B	8	38.365	47.500	76.417	1.00	8.68
6063	CD1	ILE	B	8	38.032	46.195	77.148	1.00	9.29
6067	CG2	ILE	B	8	40.190	48.301	77.980	1.00	8.89
6071	C	ILE	B	8	39.334	50.359	75.941	1.00	8.15
6072	O	ILE	B	8	39.769	51.170	76.759	1.00	8.02
6073	N	SER	B	9	38.178	50.509	75.303	1.00	7.95
6075	CA	SER	B	9	37.270	51.626	75.547	1.00	7.81
6077	CB	ASER	B	9	37.628	52.800	74.644	0.65	7.88
6080	OG	ASER	B	9	37.584	52.403	73.279	0.65	8.76
6082	C	SER	B	9	35.840	51.193	75.250	1.00	7.48
6083	O	SER	B	9	35.611	50.126	74.683	1.00	7.14
6084	N	PHE	B	10	34.878	52.014	75.644	1.00	7.33
6086	CA	PHE	B	10	33.505	51.794	75.212	1.00	7.53
6088	CB	PHE	B	10	32.712	50.997	76.261	1.00	7.38
6091	CG	PHE	B	10	32.279	51.799	77.456	1.00	7.52
6092	CD1	PHE	B	10	33.105	51.923	78.565	1.00	7.28
6094	CE1	PHE	B	10	32.701	52.644	79.676	1.00	7.36
6096	CZ	PHE	B	10	31.459	53.243	79.698	1.00	7.81
6098	CE2	PHE	B	10	30.612	53.114	78.608	1.00	7.86
6100	CD2	PHE	B	10	31.023	52.392	77.493	1.00	8.08
6102	C	PHE	B	10	32.801	53.085	74.826	1.00	7.53
6103	O	PHE	B	10	33.248	54.184	75.149	1.00	7.64
6104	N	PHE	B	11	31.713	52.921	74.089	1.00	7.82

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6106	CA	PHE	B	11	30.830	54.013	73.730	1.00	7.90
6108	CB	PHE	B	11	31.062	54.452	72.282	1.00	8.05
6111	CG	PHE	B	11	30.176	55.590	71.851	1.00	8.85
6112	CD1	PHE	B	11	30.498	56.900	72.184	1.00	10.21
6114	CE1	PHE	B	11	29.678	57.954	71.799	1.00	10.00
6116	CZ	PHE	B	11	28.518	57.700	71.087	1.00	10.09
6118	CE2	PHE	B	11	28.181	56.396	70.758	1.00	10.00
6120	CD2	PHE	B	11	29.005	55.349	71.142	1.00	9.45
6122	C	PHE	B	11	29.391	53.546	73.903	1.00	7.88
6123	O	PHE	B	11	29.044	52.415	73.572	1.00	7.64
6124	N	VAL	B	12	28.559	54.424	74.439	1.00	7.67
6126	CA	VAL	B	12	27.122	54.190	74.476	1.00	7.66
6128	CB	VAL	B	12	26.623	53.899	75.910	1.00	7.44
6130	CG1	VAL	B	12	27.199	52.585	76.409	1.00	7.66
6134	CG2	VAL	B	12	26.974	55.035	76.870	1.00	7.50
6138	C	VAL	B	12	26.438	55.420	73.894	1.00	7.74
6139	O	VAL	B	12	27.006	56.512	73.931	1.00	7.70
6140	N	PRO	B	13	25.234	55.258	73.345	1.00	8.04
6141	CA	PRO	B	13	24.516	56.398	72.766	1.00	8.23
6143	CB	PRO	B	13	23.212	55.779	72.250	1.00	8.12
6146	CG	PRO	B	13	23.084	54.477	72.956	1.00	8.19
6149	CD	PRO	B	13	24.474	54.004	73.218	1.00	7.96
6152	C	PRO	B	13	24.236	57.505	73.793	1.00	8.35
6153	O	PRO	B	13	24.266	57.249	75.002	1.00	8.43
6154	N	PRO	B	14	23.991	58.723	73.320	1.00	8.55
6155	CA	PRO	B	14	23.799	59.870	74.218	1.00	8.72
6157	CB	PRO	B	14	24.046	61.080	73.297	1.00	8.86
6160	CG	PRO	B	14	23.756	60.602	71.920	1.00	8.88
6163	CD	PRO	B	14	23.923	59.113	71.899	1.00	8.58
6166	C	PRO	B	14	22.420	59.958	74.882	1.00	8.78
6167	O	PRO	B	14	22.063	61.045	75.316	1.00	9.11
6168	N	TYR	B	15	21.674	58.856	74.967	1.00	8.86
6170	CA	TYR	B	15	20.357	58.848	75.608	1.00	8.89
6172	CB	TYR	B	15	19.237	58.854	74.552	1.00	9.12
6175	CG	TYR	B	15	19.435	59.870	73.455	1.00	10.12
6176	CD1	TYR	B	15	19.161	61.213	73.675	1.00	11.31
6178	CE1	TYR	B	15	19.359	62.162	72.681	1.00	12.15
6180	CZ	TYR	B	15	19.834	61.772	71.447	1.00	12.28
6181	OH	TYR	B	15	20.022	62.721	70.464	1.00	12.56
6183	CE2	TYR	B	15	20.120	60.437	71.199	1.00	11.49
6185	CD2	TYR	B	15	19.919	59.493	72.204	1.00	11.10
6187	C	TYR	B	15	20.172	57.636	76.517	1.00	8.63
6188	O	TYR	B	15	20.785	56.590	76.314	1.00	8.71
6189	N	TYR	B	16	19.320	57.790	77.522	1.00	8.11
6191	CA	TYR	B	16	18.926	56.675	78.373	1.00	7.89
6193	CB	TYR	B	16	19.940	56.481	79.511	1.00	7.84
6196	CG	TYR	B	16	19.954	57.597	80.542	1.00	7.55
6197	CD1	TYR	B	16	19.266	57.471	81.746	1.00	7.48
6199	CE1	TYR	B	16	19.276	58.493	82.693	1.00	7.33
6201	CZ	TYR	B	16	19.986	59.649	82.441	1.00	7.17
6202	OH	TYR	B	16	20.005	60.663	83.373	1.00	6.75
6204	CE2	TYR	B	16	20.679	59.794	81.253	1.00	7.64
6206	CD2	TYR	B	16	20.663	58.770	80.315	1.00	7.44

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6208	C	TYR	B	16	17.532	56.897	78.946	1.00	7.76
6209	O	TYR	B	16	17.000	57.997	78.871	1.00	7.36
6210	N	ILE	B	17	16.938	55.849	79.503	1.00	7.79
6212	CA	ILE	B	17	15.757	56.012	80.340	1.00	7.84
6214	CB	ILE	B	17	14.510	55.273	79.776	1.00	7.99
6216	CG1	ILE	B	17	14.793	53.789	79.517	1.00	7.93
6219	CD1	ILE	B	17	13.543	52.982	79.254	1.00	8.24
6223	CG2	ILE	B	17	14.013	55.947	78.506	1.00	7.85
6227	C	ILE	B	17	16.060	55.533	81.745	1.00	8.17
6228	O	ILE	B	17	16.910	54.663	81.957	1.00	8.10
6229	N	ASP	B	18	15.350	56.117	82.698	1.00	8.20
6231	CA	ASP	B	18	15.410	55.714	84.090	1.00	8.49
6233	CB	ASP	B	18	14.943	56.870	84.968	1.00	8.42
6236	CG	ASP	B	18	14.947	56.519	86.431	1.00	8.88
6237	OD1	ASP	B	18	13.911	56.026	86.907	1.00	8.51
6238	OD2	ASP	B	18	15.935	56.691	87.174	1.00	8.45
6239	C	ASP	B	18	14.513	54.492	84.284	1.00	8.59
6240	O	ASP	B	18	13.387	54.470	83.801	1.00	8.47
6241	N	MSE	B	19	15.005	53.486	85.001	1.00	9.04
6243	CA	MSE	B	19	14.304	52.202	85.095	1.00	9.46
6245	CB	MSE	B	19	15.270	51.072	85.471	1.00	9.51
6248	CG	MSE	B	19	16.269	50.745	84.370	1.00	10.48
6251	SE	MSE	B	19	15.462	50.056	82.750	1.00	12.23
6252	CE	MSE	B	19	14.963	48.288	83.376	1.00	11.07
6256	C	MSE	B	19	13.124	52.234	86.055	1.00	9.55
6257	O	MSE	B	19	12.196	51.445	85.904	1.00	9.59
6258	N	THR	B	20	13.155	53.122	87.045	1.00	9.67
6260	CA	THR	B	20	11.965	53.372	87.865	1.00	10.06
6262	CB	THR	B	20	12.257	54.357	89.018	1.00	10.21
6264	OG1	THR	B	20	12.942	53.675	90.063	1.00	11.41
6266	CG2	THR	B	20	10.970	54.830	89.706	1.00	10.83
6270	C	THR	B	20	10.849	53.923	86.992	1.00	9.83
6271	O	THR	B	20	9.705	53.511	87.122	1.00	9.82
6272	N	ALA	B	21	11.194	54.847	86.101	1.00	9.81
6274	CA	ALA	B	21	10.219	55.443	85.196	1.00	9.87
6276	CB	ALA	B	21	10.837	56.595	84.421	1.00	9.90
6280	C	ALA	B	21	9.644	54.397	84.242	1.00	9.88
6281	O	ALA	B	21	8.459	54.438	83.938	1.00	9.92
6282	N	LEU	B	22	10.468	53.455	83.784	1.00	9.90
6284	CA	LEU	B	22	9.968	52.381	82.927	1.00	10.02
6286	CB	LEU	B	22	11.098	51.513	82.359	1.00	9.81
6289	CG	LEU	B	22	10.619	50.459	81.342	1.00	9.32
6291	CD1	LEU	B	22	10.072	51.120	80.085	1.00	8.62
6295	CD2	LEU	B	22	11.723	49.460	80.989	1.00	8.55
6299	C	LEU	B	22	8.993	51.506	83.704	1.00	10.37
6300	O	LEU	B	22	7.937	51.161	83.192	1.00	10.52
6301	N	ALA	B	23	9.355	51.154	84.935	1.00	10.74
6303	CA	ALA	B	23	8.506	50.332	85.791	1.00	11.16
6305	CB	ALA	B	23	9.191	50.074	87.130	1.00	11.15
6309	C	ALA	B	23	7.146	50.990	86.006	1.00	11.59
6310	O	ALA	B	23	6.111	50.334	85.908	1.00	11.65
6311	N	GLU	B	24	7.160	52.290	86.271	1.00	12.27
6313	CA	GLU	B	24	5.939	53.060	86.498	1.00	13.20

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6315	CB	GLU	B	24	6.284	54.497	86.914	1.00	13.42
6318	CG	GLU	B	24	6.883	54.580	88.315	1.00	15.95
6321	CD	GLU	B	24	7.415	55.958	88.692	1.00	18.51
6322	OE1	GLU	B	24	7.059	56.436	89.788	1.00	21.38
6323	OE2	GLU	B	24	8.207	56.558	87.925	1.00	19.65
6324	C	GLU	B	24	5.036	53.045	85.262	1.00	13.23
6325	O	GLU	B	24	3.828	52.852	85.377	1.00	13.34
6326	N	ALA	B	25	5.634	53.216	84.085	1.00	13.44
6328	CA	ALA	B	25	4.892	53.205	82.821	1.00	13.59
6330	CB	ALA	B	25	5.781	53.698	81.684	1.00	13.63
6334	C	ALA	B	25	4.349	51.816	82.492	1.00	13.79
6335	O	ALA	B	25	3.272	51.687	81.905	1.00	13.63
6336	N	ARG	B	26	5.090	50.785	82.895	1.00	13.92
6338	CA	ARG	B	26	4.747	49.400	82.583	1.00	14.23
6340	CB	ARG	B	26	6.028	48.582	82.394	1.00	14.26
6343	CG	ARG	B	26	6.818	48.960	81.159	1.00	14.12
6346	CD	ARG	B	26	6.261	48.381	79.870	1.00	13.76
6349	NE	ARG	B	26	6.948	48.934	78.704	1.00	12.68
6351	CZ	ARG	B	26	6.620	50.067	78.086	1.00	13.15
6352	NH1	ARG	B	26	7.330	50.453	77.036	1.00	12.91
6355	NH2	ARG	B	26	5.612	50.829	78.509	1.00	12.84
6358	C	ARG	B	26	3.881	48.735	83.655	1.00	14.61
6359	O	ARG	B	26	3.555	47.555	83.536	1.00	14.48
6360	N	ASN	B	27	3.515	49.483	84.697	1.00	15.05
6362	CA	ASN	B	27	2.734	48.944	85.814	1.00	15.63
6364	CB	ASN	B	27	1.288	48.638	85.382	1.00	15.92
6367	CG	ASN	B	27	0.474	49.902	85.105	1.00	17.74
6368	OD1	ASN	B	27	0.580	50.901	85.822	1.00	19.96
6369	ND2	ASN	B	27	-0.359	49.851	84.073	1.00	20.56
6372	C	ASN	B	27	3.392	47.713	86.450	1.00	15.59
6373	O	ASN	B	27	2.729	46.722	86.770	1.00	15.31
6374	N	VAL	B	28	4.708	47.781	86.614	1.00	15.63
6376	CA	VAL	B	28	5.440	46.773	87.366	1.00	15.59
6378	CB	VAL	B	28	6.421	45.948	86.468	1.00	15.89
6380	CG1	VAL	B	28	5.920	45.858	85.022	1.00	16.07
6384	CG2	VAL	B	28	7.837	46.486	86.511	1.00	16.02
6388	C	VAL	B	28	6.162	47.423	88.550	1.00	15.44
6389	O	VAL	B	28	6.508	48.602	88.519	1.00	15.06
6390	N	ASP	B	29	6.344	46.628	89.598	1.00	15.37
6392	CA	ASP	B	29	7.125	46.990	90.778	1.00	15.46
6394	CB	ASP	B	29	7.243	45.750	91.674	1.00	15.86
6397	CG	ASP	B	29	7.440	46.088	93.128	1.00	17.63
6398	OD1	ASP	B	29	8.276	46.962	93.437	1.00	19.48
6399	OD2	ASP	B	29	6.809	45.508	94.038	1.00	20.82
6400	C	ASP	B	29	8.532	47.477	90.393	1.00	14.68
6401	O	ASP	B	29	9.284	46.725	89.775	1.00	14.52
6402	N	PRO	B	30	8.891	48.716	90.737	1.00	13.88
6403	CA	PRO	B	30	10.261	49.209	90.513	1.00	13.41
6405	CB	PRO	B	30	10.274	50.549	91.254	1.00	13.40
6408	CG	PRO	B	30	8.859	51.004	91.202	1.00	13.77
6411	CD	PRO	B	30	8.034	49.757	91.337	1.00	14.11
6414	C	PRO	B	30	11.342	48.274	91.065	1.00	12.95

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6415	O	PRO	B	30	12.424	48.168	90.487	1.00	12.69
6416	N	GLY	B	31	11.042	47.612	92.176	1.00	12.39
6418	CA	GLY	B	31	11.903	46.585	92.732	1.00	12.09
6421	C	GLY	B	31	12.256	45.436	91.797	1.00	11.76
6422	O	GLY	B	31	13.355	44.900	91.871	1.00	11.54
6423	N	LYS	B	32	11.330	45.034	90.934	1.00	11.49
6425	CA	LYS	B	32	11.625	44.015	89.921	1.00	11.51
6427	CB	LYS	B	32	10.413	43.752	89.020	1.00	11.58
6430	CG	LYS	B	32	10.696	42.735	87.918	1.00	12.00
6433	CD	LYS	B	32	9.430	42.254	87.231	1.00	12.94
6436	CE	LYS	B	32	9.750	41.096	86.288	1.00	13.25
6439	NZ	LYS	B	32	8.601	40.734	85.416	1.00	13.34
6443	C	LYS	B	32	12.831	44.387	89.050	1.00	11.32
6444	O	LYS	B	32	13.665	43.542	88.752	1.00	10.69
6445	N	PHE	B	33	12.904	45.644	88.632	1.00	11.40
6447	CA	PHE	B	33	14.000	46.103	87.786	1.00	11.57
6449	CB	PHE	B	33	13.574	47.334	86.975	1.00	11.68
6452	CG	PHE	B	33	12.482	47.066	85.954	1.00	11.23
6453	CD1	PHE	B	33	12.030	45.772	85.676	1.00	11.28
6455	CE1	PHE	B	33	11.035	45.555	84.731	1.00	10.87
6457	CZ	PHE	B	33	10.474	46.624	84.052	1.00	10.60
6459	CE2	PHE	B	33	10.908	47.911	84.319	1.00	11.10
6461	CD2	PHE	B	33	11.903	48.127	85.265	1.00	11.53
6463	C	PHE	B	33	15.259	46.395	88.608	1.00	11.99
6464	O	PHE	B	33	16.356	45.999	88.223	1.00	11.67
6465	N	HIS	B	34	15.095	47.043	89.756	1.00	12.14
6467	CA	HIS	B	34	16.233	47.505	90.556	1.00	12.63
6469	CB	BHIS	B	34	15.725	48.534	91.576	0.35	12.50
6470	CB	AHIS	B	34	15.821	48.620	91.514	0.65	12.74
6475	CG	BHIS	B	34	16.804	49.212	92.361	0.35	12.42
6476	CG	AHIS	B	34	15.697	49.944	90.835	0.65	13.74
6477	ND1	BHIS	B	34	16.967	49.027	93.716	0.35	12.36
6478	ND1	AHIS	B	34	14.564	50.722	90.908	0.65	14.45
6481	CE1	BHIS	B	34	17.982	49.758	94.140	0.35	12.26
6482	CE1	AHIS	B	34	14.743	51.815	90.190	0.65	15.15
6485	NE2	BHIS	B	34	18.479	50.416	93.108	0.35	12.76
6486	NE2	AHIS	B	34	15.939	51.765	89.637	0.65	15.08
6489	CD2	BHIS	B	34	17.756	50.096	91.986	0.35	12.36
6490	CD2	AHIS	B	34	16.554	50.602	90.020	0.65	13.99
6493	C	HIS	B	34	16.971	46.379	91.280	1.00	12.66
6494	O	HIS	B	34	18.198	46.399	91.350	1.00	12.36
6495	N	ILE	B	35	16.227	45.400	91.788	1.00	12.80
6497	CA	ILE	B	35	16.808	44.250	92.481	1.00	13.30
6499	CB	ILE	B	35	16.161	44.080	93.876	1.00	13.38
6501	CG1	ILE	B	35	16.474	45.304	94.751	1.00	14.39
6504	CD1	ILE	B	35	15.730	45.359	96.096	1.00	15.65
6508	CG2	ILE	B	35	16.651	42.794	94.548	1.00	14.03
6512	C	ILE	B	35	16.682	42.955	91.667	1.00	13.23
6513	O	ILE	B	35	17.653	42.220	91.526	1.00	13.45
6514	N	GLY	B	36	15.492	42.676	91.140	1.00	13.20
6516	CA	GLY	B	36	15.232	41.418	90.454	1.00	13.18
6519	C	GLY	B	36	16.115	41.193	89.242	1.00	13.27

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6520	O	GLY	B	36	16.674	40.115	89.064	1.00	13.07
6521	N	ILE	B	37	16.252	42.231	88.425	1.00	13.44
6523	CA	ILE	B	37	17.077	42.190	87.220	1.00	13.85
6525	CB	ILE	B	37	16.247	42.747	86.033	1.00	14.28
6527	CG1	ILE	B	37	15.123	41.760	85.695	1.00	15.96
6530	CD1	ILE	B	37	13.940	42.399	84.989	1.00	17.56
6534	CG2	ILE	B	37	17.087	42.978	84.796	1.00	15.32
6538	C	ILE	B	37	18.393	42.951	87.461	1.00	13.29
6539	O	ILE	B	37	19.441	42.554	86.960	1.00	13.28
6540	N	GLY	B	38	18.338	44.017	88.260	1.00	12.52
6542	CA	GLY	B	38	19.523	44.768	88.648	1.00	11.90
6545	C	GLY	B	38	19.921	45.898	87.711	1.00	11.34
6546	O	GLY	B	38	21.105	46.093	87.452	1.00	11.12
6547	N	GLN	B	39	18.941	46.658	87.226	1.00	10.97
6549	CA	GLN	B	39	19.182	47.751	86.287	1.00	10.82
6551	CB	GLN	B	39	18.564	47.420	84.930	1.00	10.92
6554	CG	GLN	B	39	19.050	46.128	84.303	1.00	11.21
6557	CD	GLN	B	39	20.552	46.072	84.101	1.00	11.92
6558	OE1	GLN	B	39	21.165	45.047	84.360	1.00	14.41
6559	NE2	GLN	B	39	21.141	47.161	83.628	1.00	11.68
6562	C	GLN	B	39	18.608	49.077	86.780	1.00	10.71
6563	O	GLN	B	39	17.505	49.119	87.333	1.00	10.50
6564	N	ASP	B	40	19.365	50.150	86.546	1.00	10.36
6566	CA	ASP	B	40	19.015	51.505	86.965	1.00	10.24
6568	CB	ASP	B	40	20.145	52.103	87.805	1.00	10.33
6571	CG	ASP	B	40	20.395	51.330	89.079	1.00	10.61
6572	OD1	ASP	B	40	21.547	51.294	89.549	1.00	10.78
6573	OD2	ASP	B	40	19.492	50.732	89.680	1.00	9.84
6574	C	ASP	B	40	18.739	52.440	85.788	1.00	9.86
6575	O	ASP	B	40	17.826	53.254	85.854	1.00	9.83
6576	N	GLN	B	41	19.547	52.346	84.734	1.00	9.64
6578	CA	GLN	B	41	19.365	53.147	83.515	1.00	9.47
6580	CB	GLN	B	41	20.274	54.385	83.532	1.00	9.36
6583	CG	GLN	B	41	20.121	55.274	84.767	1.00	9.47
6586	CD	GLN	B	41	21.235	56.301	84.916	1.00	9.49
6587	OE1	GLN	B	41	22.358	56.077	84.468	1.00	9.00
6588	NE2	GLN	B	41	20.926	57.419	85.560	1.00	8.91
6591	C	GLN	B	41	19.662	52.304	82.266	1.00	9.36
6592	O	GLN	B	41	20.595	51.493	82.269	1.00	9.52
6593	N	MSE	B	42	18.868	52.501	81.212	1.00	9.19
6595	CA	MSE	B	42	18.996	51.752	79.954	1.00	8.73
6597	CB	MSE	B	42	17.665	51.075	79.593	1.00	8.52
6600	CG	MSE	B	42	17.507	50.691	78.114	0.65	7.15
6603	SE	MSE	B	42	15.656	50.495	77.556	0.65	5.04
6604	CE	MSE	B	42	15.129	49.260	78.919	0.65	3.30
6608	C	MSE	B	42	19.406	52.675	78.810	1.00	9.03
6609	O	MSE	B	42	18.738	53.670	78.540	1.00	8.87
6610	N	ALA	B	43	20.488	52.314	78.126	1.00	9.15
6612	CA	ALA	B	43	20.929	53.001	76.914	1.00	9.35
6614	CB	ALA	B	43	22.295	52.478	76.489	1.00	9.28
6618	C	ALA	B	43	19.926	52.814	75.776	1.00	9.74
6619	O	ALA	B	43	19.431	51.710	75.549	1.00	9.76

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6620	N	VAL	B	44	19.630	53.905	75.073	1.00	9.98
6622	CA	VAL	B	44	18.722	53.895	73.927	1.00	10.30
6624	CB	VAL	B	44	17.299	54.355	74.336	1.00	10.48
6626	CG1	VAL	B	44	16.358	54.402	73.126	1.00	11.30
6630	CG2	VAL	B	44	16.732	53.413	75.391	1.00	10.90
6634	C	VAL	B	44	19.294	54.799	72.833	1.00	10.31
6635	O	VAL	B	44	20.013	55.758	73.124	1.00	10.12
6636	N	ASN	B	45	18.997	54.472	71.577	1.00	10.43
6638	CA	ASN	B	45	19.539	55.210	70.438	1.00	10.61
6640	CB	ASN	B	45	20.759	54.490	69.853	1.00	10.51
6643	CG	ASN	B	45	20.416	53.141	69.252	1.00	10.59
6644	OD1	ASN	B	45	20.312	52.146	69.966	1.00	10.53
6645	ND2	ASN	B	45	20.231	53.103	67.932	1.00	9.40
6648	C	ASN	B	45	18.511	55.456	69.340	1.00	10.98
6649	O	ASN	B	45	17.579	54.663	69.152	1.00	10.53
6650	N	PRO	B	46	18.688	56.550	68.603	1.00	11.26
6651	CA	PRO	B	46	17.811	56.844	67.476	1.00	11.44
6653	CB	PRO	B	46	18.060	58.333	67.225	1.00	11.44
6656	CG	PRO	B	46	19.470	58.531	67.610	1.00	11.39
6659	CD	PRO	B	46	19.721	57.588	68.764	1.00	11.19
6662	C	PRO	B	46	18.222	56.017	66.275	1.00	11.68
6663	O	PRO	B	46	19.304	55.422	66.251	1.00	11.73
6664	N	ILE	B	47	17.365	56.018	65.269	1.00	11.77
6666	CA	ILE	B	47	17.554	55.208	64.081	1.00	12.10
6668	CB	ILE	B	47	16.203	55.128	63.321	1.00	12.50
6670	CG1	ILE	B	47	16.154	53.885	62.437	1.00	14.50
6673	CD1	ILE	B	47	15.948	52.573	63.186	1.00	15.85
6677	CG2	ILE	B	47	15.935	56.415	62.519	1.00	13.10
6681	C	ILE	B	47	18.706	55.746	63.206	1.00	11.34
6682	O	ILE	B	47	19.190	55.068	62.303	1.00	11.58
6683	N	SER	B	48	19.148	56.965	63.503	1.00	10.49
6685	CA	SER	B	48	20.323	57.558	62.876	1.00	9.76
6687	CB	SER	B	48	20.254	59.080	63.034	1.00	9.85
6690	OG	SER	B	48	20.140	59.435	64.399	1.00	8.56
6692	C	SER	B	48	21.668	57.050	63.426	1.00	9.36
6693	O	SER	B	48	22.719	57.534	63.023	1.00	9.52
6694	N	GLN	B	49	21.638	56.085	64.338	1.00	8.82
6696	CA	GLN	B	49	22.850	55.514	64.925	1.00	8.17
6698	CB	GLN	B	49	22.983	55.959	66.384	1.00	8.26
6701	CG	GLN	B	49	23.162	57.473	66.547	1.00	7.72
6704	CD	GLN	B	49	23.127	57.937	67.996	1.00	8.24
6705	OE1	GLN	B	49	23.383	57.156	68.918	1.00	6.37
6706	NE2	GLN	B	49	22.804	59.215	68.201	1.00	8.63
6709	C	GLN	B	49	22.793	53.991	64.831	1.00	8.00
6710	O	GLN	B	49	21.829	53.377	65.281	1.00	7.70
6711	N	ASP	B	50	23.814	53.391	64.223	1.00	7.86
6713	CA	ASP	B	50	23.882	51.939	64.043	1.00	7.79
6715	CB	ASP	B	50	23.682	51.580	62.558	1.00	7.84
6718	CG	ASP	B	50	24.803	52.085	61.667	1.00	7.80
6719	OD1	ASP	B	50	24.616	52.112	60.426	1.00	8.06
6720	OD2	ASP	B	50	25.899	52.480	62.108	1.00	6.46
6721	C	ASP	B	50	25.200	51.387	64.604	1.00	7.72

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6722	O	ASP	B	50	25.930	52.106	65.283	1.00	7.78
6723	N	ILE	B	51	25.508	50.123	64.324	1.00	7.46
6725	CA	ILE	B	51	26.715	49.507	64.876	1.00	7.43
6727	CB	ILE	B	51	26.766	47.983	64.626	1.00	7.67
6729	CG1	ILE	B	51	26.566	47.642	63.142	1.00	7.53
6732	CD1	ILE	B	51	27.045	46.271	62.792	1.00	8.04
6736	CG2	ILE	B	51	25.743	47.263	65.505	1.00	7.52
6740	C	ILE	B	51	28.000	50.174	64.391	1.00	7.20
6741	O	ILE	B	51	28.976	50.207	65.129	1.00	6.95
6742	N	VAL	B	52	27.993	50.712	63.170	1.00	7.05
6744	CA	VAL	B	52	29.133	51.476	62.650	1.00	7.13
6746	CB	VAL	B	52	28.971	51.846	61.146	1.00	7.10
6748	CG1	VAL	B	52	30.128	52.734	60.676	1.00	7.56
6752	CG2	VAL	B	52	28.893	50.590	60.289	1.00	7.18
6756	C	VAL	B	52	29.344	52.754	63.462	1.00	6.97
6757	O	VAL	B	52	30.466	53.085	63.820	1.00	7.05
6758	N	THR	B	53	28.266	53.470	63.750	1.00	7.20
6760	CA	THR	B	53	28.332	54.653	64.609	1.00	7.34
6762	CB	THR	B	53	26.914	55.181	64.912	1.00	7.40
6764	OG1	THR	B	53	26.206	55.437	63.688	1.00	7.94
6766	CG2	THR	B	53	26.979	56.532	65.614	1.00	7.28
6770	C	THR	B	53	29.035	54.359	65.934	1.00	7.35
6771	O	THR	B	53	29.962	55.062	66.325	1.00	7.11
6772	N	PHE	B	54	28.582	53.317	66.617	1.00	7.48
6774	CA	PHE	B	54	29.117	52.972	67.929	1.00	7.73
6776	CB	PHE	B	54	28.218	51.942	68.624	1.00	7.88
6779	CG	PHE	B	54	26.790	52.403	68.821	1.00	9.16
6780	CD1	PHE	B	54	25.773	51.474	68.965	1.00	10.57
6782	CE1	PHE	B	54	24.462	51.884	69.152	1.00	11.25
6784	CZ	PHE	B	54	24.155	53.229	69.191	1.00	11.34
6786	CE2	PHE	B	54	25.155	54.166	69.052	1.00	11.04
6788	CD2	PHE	B	54	26.463	53.757	68.866	1.00	9.97
6790	C	PHE	B	54	30.545	52.455	67.835	1.00	7.63
6791	O	PHE	B	54	31.387	52.820	68.650	1.00	7.58
6792	N	ALA	B	55	30.815	51.615	66.839	1.00	7.64
6794	CA	ALA	B	55	32.141	51.032	66.651	1.00	7.62
6796	CB	ALA	B	55	32.110	49.992	65.552	1.00	7.58
6800	C	ALA	B	55	33.184	52.098	66.333	1.00	7.66
6801	O	ALA	B	55	34.303	52.045	66.841	1.00	7.81
6802	N	ALA	B	56	32.813	53.064	65.497	1.00	7.59
6804	CA	ALA	B	56	33.728	54.135	65.101	1.00	7.91
6806	CB	ALA	B	56	33.148	54.929	63.936	1.00	7.75
6810	C	ALA	B	56	34.038	55.062	66.274	1.00	7.94
6811	O	ALA	B	56	35.176	55.482	66.450	1.00	7.82
6812	N	ASN	B	57	33.019	55.379	67.071	1.00	8.07
6814	CA	ASN	B	57	33.197	56.225	68.251	1.00	8.28
6816	CB	ASN	B	57	31.840	56.693	68.805	1.00	8.08
6819	CG	ASN	B	57	31.311	57.929	68.083	1.00	8.68
6820	OD1	ASN	B	57	31.813	59.033	68.282	1.00	9.61
6821	ND2	ASN	B	57	30.298	57.744	67.242	1.00	7.87
6824	C	ASN	B	57	34.033	55.527	69.336	1.00	8.28
6825	O	ASN	B	57	34.891	56.148	69.948	1.00	8.32

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6826	N	ALA	B	58	33.817	54.233	69.541	1.00	8.45
6828	CA	ALA	B	58	34.586	53.478	70.535	1.00	8.58
6830	CB	ALA	B	58	33.991	52.095	70.739	1.00	8.59
6834	C	ALA	B	58	36.054	53.365	70.146	1.00	8.74
6835	O	ALA	B	58	36.940	53.600	70.970	1.00	8.79
6836	N	ALA	B	59	36.299	52.994	68.892	1.00	8.94
6838	CA	ALA	B	59	37.651	52.820	68.374	1.00	9.30
6840	CB	ALA	B	59	37.612	52.155	67.003	1.00	9.25
6844	C	ALA	B	59	38.429	54.138	68.299	1.00	9.81
6845	O	ALA	B	59	39.644	54.146	68.475	1.00	9.51
6846	N	GLU	B	60	37.733	55.243	68.038	1.00	10.12
6848	CA	GLU	B	60	38.372	56.562	68.000	1.00	10.75
6850	CB	GLU	B	60	37.358	57.655	67.646	1.00	11.06
6853	CG	GLU	B	60	37.936	59.059	67.660	1.00	13.54
6856	CD	GLU	B	60	37.158	60.021	66.789	1.00	16.66
6857	OE1	GLU	B	60	37.106	59.812	65.559	1.00	20.20
6858	OE2	GLU	B	60	36.604	60.987	67.335	1.00	19.85
6859	C	GLU	B	60	39.037	56.891	69.337	1.00	10.37
6860	O	GLU	B	60	40.063	57.567	69.373	1.00	10.72
6861	N	ALA	B	61	38.446	56.409	70.428	1.00	10.12
6863	CA	ALA	B	61	38.985	56.632	71.769	1.00	9.80
6865	CB	ALA	B	61	38.041	56.048	72.823	1.00	9.92
6869	C	ALA	B	61	40.403	56.079	71.975	1.00	9.50
6870	O	ALA	B	61	41.159	56.628	72.772	1.00	9.14
6871	N	ILE	B	62	40.757	55.005	71.265	1.00	9.13
6873	CA	ILE	B	62	42.021	54.292	71.515	1.00	9.12
6875	CB	ILE	B	62	41.749	52.800	71.895	1.00	9.15
6877	CG1	ILE	B	62	40.879	52.102	70.850	1.00	8.64
6880	CD1	ILE	B	62	40.883	50.590	70.971	1.00	8.95
6884	CG2	ILE	B	62	41.100	52.702	73.271	1.00	9.62
6888	C	ILE	B	62	43.068	54.348	70.394	1.00	9.06
6889	O	ILE	B	62	44.258	54.198	70.668	1.00	8.87
6890	N	LEU	B	63	42.645	54.564	69.149	1.00	9.05
6892	CA	LEU	B	63	43.545	54.391	68.006	1.00	9.20
6894	CB	LEU	B	63	42.762	53.983	66.757	1.00	9.45
6897	CG	LEU	B	63	42.059	52.626	66.818	1.00	9.71
6899	CD1	LEU	B	63	41.365	52.349	65.498	1.00	10.99
6903	CD2	LEU	B	63	43.037	51.510	67.160	1.00	10.12
6907	C	LEU	B	63	44.393	55.622	67.694	1.00	9.23
6908	O	LEU	B	63	43.895	56.746	67.659	1.00	8.67
6909	N	THR	B	64	45.680	55.374	67.457	1.00	9.40
6911	CA	THR	B	64	46.633	56.391	67.032	1.00	9.49
6913	CB	THR	B	64	47.903	56.317	67.890	1.00	9.46
6915	OG1	THR	B	64	48.564	55.055	67.696	1.00	8.48
6917	CG2	THR	B	64	47.559	56.357	69.376	1.00	9.16
6921	C	THR	B	64	47.002	56.171	65.578	1.00	10.16
6922	O	THR	B	64	46.655	55.147	64.997	1.00	9.62
6923	N	LYS	B	65	47.706	57.139	64.995	1.00	10.80
6925	CA	LYS	B	65	48.255	56.999	63.645	1.00	11.52
6927	CB	LYS	B	65	49.017	58.272	63.237	1.00	11.99
6930	CG	LYS	B	65	49.892	58.125	61.995	1.00	14.05
6933	CD	LYS	B	65	50.177	59.465	61.323	1.00	16.38

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6936	CE	LYS	B	65	50.752	59.262	59.927	1.00	17.78
6939	NZ	LYS	B	65	51.451	60.487	59.448	1.00	18.55
6943	C	LYS	B	65	49.152	55.764	63.513	1.00	11.70
6944	O	LYS	B	65	49.089	55.060	62.505	1.00	11.54
6945	N	GLU	B	66	49.981	55.490	64.518	1.00	11.90
6947	CA	GLU	B	66	50.873	54.334	64.427	1.00	12.04
6949	CB	GLU	B	66	52.118	54.478	65.312	1.00	12.65
6952	CG	GLU	B	66	51.901	54.506	66.807	1.00	13.77
6955	CD	GLU	B	66	53.181	54.844	67.571	1.00	15.02
6956	OE1	GLU	B	66	54.245	55.036	66.932	1.00	16.61
6957	OE2	GLU	B	66	53.123	54.915	68.813	1.00	12.38
6958	C	GLU	B	66	50.140	53.003	64.643	1.00	11.57
6959	O	GLU	B	66	50.526	52.005	64.046	1.00	11.19
6960	N	ASP	B	67	49.074	52.991	65.446	1.00	11.03
6962	CA	ASP	B	67	48.189	51.821	65.521	1.00	10.75
6964	CB	ASP	B	67	47.003	52.057	66.462	1.00	10.68
6967	CG	ASP	B	67	47.395	52.090	67.925	1.00	9.95
6968	OD1	ASP	B	67	46.614	52.653	68.718	1.00	9.21
6969	OD2	ASP	B	67	48.436	51.579	68.379	1.00	9.31
6970	C	ASP	B	67	47.620	51.536	64.134	1.00	10.87
6971	O	ASP	B	67	47.593	50.398	63.679	1.00	10.55
6972	N	LYS	B	68	47.169	52.591	63.467	1.00	10.91
6974	CA	LYS	B	68	46.520	52.462	62.170	1.00	11.29
6976	CB	LYS	B	68	45.951	53.808	61.715	1.00	11.12
6979	CG	LYS	B	68	44.736	54.236	62.533	1.00	11.60
6982	CD	LYS	B	68	44.515	55.732	62.508	1.00	11.28
6985	CE	LYS	B	68	43.460	56.147	63.516	1.00	11.97
6988	NZ	LYS	B	68	42.820	57.437	63.132	1.00	12.27
6992	C	LYS	B	68	47.466	51.876	61.125	1.00	11.42
6993	O	LYS	B	68	47.019	51.165	60.234	1.00	11.64
6994	N	GLU	B	69	48.764	52.142	61.265	1.00	11.69
6996	CA	GLU	B	69	49.783	51.571	60.374	1.00	12.26
6998	CB	GLU	B	69	51.052	52.434	60.379	1.00	12.71
7001	CG	GLU	B	69	50.918	53.749	59.627	1.00	15.37
7004	CD	GLU	B	69	50.417	53.568	58.203	1.00	19.14
7005	OE1	GLU	B	69	50.856	52.605	57.523	1.00	21.31
7006	OE2	GLU	B	69	49.575	54.386	57.768	1.00	22.20
7007	C	GLU	B	69	50.163	50.122	60.690	1.00	11.77
7008	O	GLU	B	69	50.610	49.397	59.801	1.00	11.80
7009	N	ALA	B	70	50.004	49.709	61.946	1.00	11.28
7011	CA	ALA	B	70	50.369	48.356	62.377	1.00	10.71
7013	CB	ALA	B	70	51.005	48.404	63.760	1.00	10.67
7017	C	ALA	B	70	49.204	47.365	62.379	1.00	10.29
7018	O	ALA	B	70	49.430	46.159	62.490	1.00	9.99
7019	N	ILE	B	71	47.971	47.859	62.262	1.00	9.85
7021	CA	ILE	B	71	46.798	46.990	62.276	1.00	9.48
7023	CB	ILE	B	71	45.514	47.769	62.661	1.00	9.43
7025	CG1	ILE	B	71	45.498	48.082	64.157	1.00	9.33
7028	CD1	ILE	B	71	44.579	49.237	64.519	1.00	9.50
7032	CG2	ILE	B	71	44.260	46.969	62.297	1.00	9.37
7036	C	ILE	B	71	46.633	46.361	60.900	1.00	9.23
7037	O	ILE	B	71	46.501	47.073	59.904	1.00	8.76

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7038	N	ASP	B	72	46.637	45.031	60.850	1.00	9.13
7040	CA	ASP	B	72	46.412	44.312	59.596	1.00	9.13
7042	CB	ASP	B	72	47.695	43.601	59.140	1.00	9.36
7045	CG	ASP	B	72	48.089	42.436	60.026	1.00	9.51
7046	OD1	ASP	B	72	47.560	42.284	61.153	1.00	9.46
7047	OD2	ASP	B	72	48.949	41.611	59.654	1.00	9.56
7048	C	ASP	B	72	45.204	43.364	59.645	1.00	9.04
7049	O	ASP	B	72	45.012	42.539	58.745	1.00	9.02
7050	N	MSE	B	73	44.386	43.494	60.686	1.00	8.74
7052	CA	MSE	B	73	43.102	42.801	60.753	1.00	8.69
7054	CB	MSE	B	73	43.274	41.387	61.322	1.00	8.97
7057	CG	MSE	B	73	41.991	40.569	61.321	1.00	9.32
7060	SE	MSE	B	73	42.277	38.638	61.433	1.00	12.78
7061	CE	MSE	B	73	43.198	38.553	63.112	1.00	10.88
7065	C	MSE	B	73	42.093	43.592	61.593	1.00	8.36
7066	O	MSE	B	73	42.423	44.082	62.669	1.00	8.05
7067	N	VAL	B	74	40.872	43.718	61.074	1.00	8.04
7069	CA	VAL	B	74	39.783	44.439	61.729	1.00	7.80
7071	CB	VAL	B	74	39.376	45.701	60.930	1.00	7.72
7073	CG1	VAL	B	74	38.256	46.456	61.640	1.00	7.53
7077	CG2	VAL	B	74	40.582	46.616	60.703	1.00	8.12
7081	C	VAL	B	74	38.583	43.498	61.825	1.00	7.58
7082	O	VAL	B	74	38.098	43.015	60.810	1.00	7.50
7083	N	ILE	B	75	38.123	43.231	63.043	1.00	7.40
7085	CA	ILE	B	75	37.015	42.312	63.280	1.00	7.30
7087	CB	ILE	B	75	37.483	41.084	64.105	1.00	7.47
7089	CG1	ILE	B	75	38.602	40.332	63.377	1.00	7.67
7092	CD1	ILE	B	75	39.306	39.292	64.241	1.00	7.71
7096	CG2	ILE	B	75	36.322	40.129	64.364	1.00	7.66
7100	C	ILE	B	75	35.920	43.052	64.029	1.00	7.19
7101	O	ILE	B	75	36.193	43.734	65.014	1.00	7.34
7102	N	VAL	B	76	34.686	42.921	63.559	1.00	6.98
7104	CA	VAL	B	76	33.527	43.381	64.311	1.00	6.66
7106	CB	VAL	B	76	32.674	44.372	63.496	1.00	6.65
7108	CG1	VAL	B	76	31.329	44.646	64.187	1.00	6.47
7112	CG2	VAL	B	76	33.435	45.667	63.291	1.00	6.68
7116	C	VAL	B	76	32.701	42.164	64.706	1.00	6.55
7117	O	VAL	B	76	32.293	41.383	63.852	1.00	6.27
7118	N	GLY	B	77	32.488	41.996	66.006	1.00	6.51
7120	CA	GLY	B	77	31.551	41.017	66.524	1.00	6.42
7123	C	GLY	B	77	30.212	41.697	66.728	1.00	6.39
7124	O	GLY	B	77	30.134	42.738	67.370	1.00	6.20
7125	N	THR	B	78	29.161	41.108	66.175	1.00	6.22
7127	CA	THR	B	78	27.832	41.696	66.239	1.00	6.26
7129	CB	THR	B	78	27.747	42.926	65.281	1.00	6.20
7131	OG1	THR	B	78	26.546	43.666	65.529	1.00	5.52
7133	CG2	THR	B	78	27.643	42.502	63.810	1.00	6.26
7137	C	THR	B	78	26.739	40.680	65.903	1.00	6.54
7138	O	THR	B	78	26.990	39.658	65.268	1.00	6.66
7139	N	GLU	B	79	25.537	40.971	66.380	1.00	6.93
7141	CA	GLU	B	79	24.313	40.309	65.953	1.00	7.29
7143	CB	GLU	B	79	23.780	39.427	67.084	1.00	7.52

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7146	CG	GLU	B	79	23.394	40.183	68.346	1.00	8.01
7149	CD	GLU	B	79	22.711	39.293	69.360	1.00	8.61
7150	OE1	GLU	B	79	21.488	39.072	69.227	1.00	8.33
7151	OE2	GLU	B	79	23.402	38.815	70.281	1.00	8.46
7152	C	GLU	B	79	23.262	41.352	65.542	1.00	7.45
7153	O	GLU	B	79	22.073	41.048	65.466	1.00	7.53
7154	N	SER	B	80	23.714	42.579	65.280	1.00	7.57
7156	CA	SER	B	80	22.840	43.699	64.918	1.00	7.59
7158	CB	SER	B	80	22.947	44.810	65.970	1.00	7.65
7161	OG	SER	B	80	22.736	44.312	67.282	1.00	6.95
7163	C	SER	B	80	23.251	44.234	63.546	1.00	7.69
7164	O	SER	B	80	23.329	45.447	63.333	1.00	7.98
7165	N	SER	B	81	23.516	43.319	62.616	1.00	7.72
7167	CA	SER	B	81	24.106	43.680	61.329	1.00	7.69
7169	CB	SER	B	81	24.596	42.431	60.587	1.00	7.79
7172	OG	SER	B	81	23.518	41.597	60.200	1.00	7.75
7174	C	SER	B	81	23.146	44.481	60.448	1.00	7.61
7175	O	SER	B	81	21.927	44.420	60.616	1.00	7.37
7176	N	ILE	B	82	23.726	45.233	59.517	1.00	7.65
7178	CA	ILE	B	82	22.985	46.088	58.587	1.00	7.88
7180	CB	ILE	B	82	23.421	47.566	58.763	1.00	8.13
7182	CG1	ILE	B	82	24.941	47.719	58.610	1.00	8.23
7185	CD1	ILE	B	82	25.434	49.157	58.651	1.00	8.96
7189	CG2	ILE	B	82	22.962	48.077	60.128	1.00	8.71
7193	C	ILE	B	82	23.155	45.641	57.128	1.00	7.77
7194	O	ILE	B	82	22.549	46.207	56.219	1.00	7.67
7195	N	ASP	B	83	23.978	44.619	56.916	1.00	7.50
7197	CA	ASP	B	83	24.133	43.995	55.608	1.00	7.47
7199	CB	ASP	B	83	25.313	44.627	54.870	1.00	7.26
7202	CG	ASP	B	83	25.189	44.525	53.366	1.00	7.04
7203	OD1	ASP	B	83	24.704	45.487	52.738	1.00	6.29
7204	OD2	ASP	B	83	25.564	43.525	52.721	1.00	6.05
7205	C	ASP	B	83	24.355	42.493	55.789	1.00	7.40
7206	O	ASP	B	83	25.004	42.074	56.745	1.00	7.38
7207	N	GLU	B	84	23.819	41.699	54.863	1.00	7.39
7209	CA	GLU	B	84	23.950	40.240	54.891	1.00	7.52
7211	CB	GLU	B	84	22.767	39.589	54.165	1.00	7.49
7214	CG	GLU	B	84	21.406	39.921	54.753	1.00	7.77
7217	CD	GLU	B	84	21.231	39.412	56.171	1.00	8.17
7218	OE1	GLU	B	84	21.969	38.483	56.576	1.00	7.42
7219	OE2	GLU	B	84	20.352	39.950	56.880	1.00	8.27
7220	C	GLU	B	84	25.249	39.733	54.261	1.00	7.54
7221	O	GLU	B	84	25.604	38.567	54.436	1.00	7.76
7222	N	SER	B	85	25.945	40.610	53.535	1.00	7.44
7224	CA	SER	B	85	27.158	40.254	52.802	1.00	7.23
7226	CB	SER	B	85	26.921	40.453	51.302	1.00	7.35
7229	OG	SER	B	85	28.117	40.312	50.556	1.00	7.16
7231	C	SER	B	85	28.358	41.090	53.249	1.00	7.19
7232	O	SER	B	85	29.393	40.548	53.634	1.00	6.98
7233	N	LYS	B	86	28.216	42.410	53.185	1.00	7.33
7235	CA	LYS	B	86	29.306	43.330	53.493	1.00	7.58
7237	CB	LYS	B	86	29.030	44.702	52.869	1.00	7.63

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7240	CG	LYS	B	86	30.161	45.703	53.028	1.00	7.94
7243	CD	LYS	B	86	30.028	46.824	52.002	1.00	8.85
7246	CE	LYS	B	86	30.906	48.013	52.345	1.00	8.51
7249	NZ	LYS	B	86	31.205	48.818	51.136	1.00	8.73
7253	C	LYS	B	86	29.501	43.475	54.995	1.00	7.50
7254	O	LYS	B	86	28.592	43.906	55.708	1.00	7.54
7255	N	ALA	B	87	30.695	43.117	55.461	1.00	7.29
7257	CA	ALA	B	87	31.050	43.202	56.874	1.00	7.22
7259	CB	ALA	B	87	32.415	42.579	57.102	1.00	7.03
7263	C	ALA	B	87	31.063	44.650	57.340	1.00	7.15
7264	O	ALA	B	87	31.601	45.514	56.657	1.00	6.99
7265	N	ALA	B	88	30.493	44.907	58.514	1.00	7.30
7267	CA	ALA	B	88	30.564	46.232	59.130	1.00	7.23
7269	CB	ALA	B	88	29.831	46.232	60.465	1.00	7.30
7273	C	ALA	B	88	32.018	46.670	59.328	1.00	7.18
7274	O	ALA	B	88	32.315	47.864	59.318	1.00	7.50
7275	N	ALA	B	89	32.917	45.701	59.506	1.00	6.97
7277	CA	ALA	B	89	34.344	45.968	59.696	1.00	6.83
7279	CB	ALA	B	89	35.089	44.663	59.981	1.00	6.97
7283	C	ALA	B	89	34.998	46.691	58.516	1.00	6.89
7284	O	ALA	B	89	35.982	47.398	58.698	1.00	6.86
7285	N	VAL	B	90	34.468	46.486	57.312	1.00	7.09
7287	CA	VAL	B	90	34.972	47.157	56.117	1.00	7.12
7289	CB	VAL	B	90	34.313	46.611	54.838	1.00	7.21
7291	CG1	VAL	B	90	34.705	47.461	53.627	1.00	7.23
7295	CG2	VAL	B	90	34.704	45.144	54.623	1.00	7.18
7299	C	VAL	B	90	34.752	48.667	56.205	1.00	7.21
7300	O	VAL	B	90	35.662	49.449	55.922	1.00	7.09
7301	N	VAL	B	91	33.549	49.070	56.603	1.00	7.34
7303	CA	VAL	B	91	33.249	50.490	56.781	1.00	7.42
7305	CB	VAL	B	91	31.741	50.737	57.004	1.00	7.45
7307	CG1	VAL	B	91	31.463	52.234	57.152	1.00	7.31
7311	CG2	VAL	B	91	30.937	50.151	55.856	1.00	7.57
7315	C	VAL	B	91	34.059	51.068	57.949	1.00	7.42
7316	O	VAL	B	91	34.577	52.175	57.861	1.00	7.48
7317	N	LEU	B	92	34.175	50.312	59.035	1.00	7.65
7319	CA	LEU	B	92	35.010	50.719	60.168	1.00	7.86
7321	CB	LEU	B	92	34.925	49.686	61.288	1.00	8.01
7324	CG	LEU	B	92	35.699	49.963	62.575	1.00	8.20
7326	CD1	LEU	B	92	35.213	51.243	63.237	1.00	8.64
7330	CD2	LEU	B	92	35.561	48.783	63.519	1.00	8.52
7334	C	LEU	B	92	36.475	50.936	59.754	1.00	7.96
7335	O	LEU	B	92	37.108	51.897	60.181	1.00	7.93
7336	N	HIS	B	93	36.998	50.042	58.922	1.00	8.02
7338	CA	HIS	B	93	38.373	50.129	58.434	1.00	8.16
7340	CB	HIS	B	93	38.669	48.947	57.501	1.00	8.37
7343	CG	HIS	B	93	40.000	49.023	56.817	1.00	8.87
7344	ND1	HIS	B	93	40.201	49.743	55.659	1.00	9.04
7346	CE1	HIS	B	93	41.463	49.628	55.285	1.00	8.95
7348	NE2	HIS	B	93	42.088	48.857	56.157	1.00	8.12
7350	CD2	HIS	B	93	41.194	48.461	57.123	1.00	8.80
7352	C	HIS	B	93	38.613	51.468	57.721	1.00	8.22

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7353	O	HIS	B	93	39.650	52.103	57.915	1.00	8.01
7354	N	ARG	B	94	37.649	51.895	56.910	1.00	8.13
7356	CA	ARG	B	94	37.728	53.190	56.232	1.00	8.47
7358	CB	ARG	B	94	36.595	53.345	55.213	1.00	8.47
7361	CG	ARG	B	94	36.543	54.729	54.545	1.00	9.24
7364	CD	ARG	B	94	35.476	54.863	53.479	1.00	9.63
7367	NE	ARG	B	94	34.130	54.799	54.053	1.00	10.38
7369	CZ	ARG	B	94	33.479	55.833	54.590	1.00	10.84
7370	NH1	ARG	B	94	32.257	55.658	55.079	1.00	10.90
7373	NH2	ARG	B	94	34.040	57.031	54.667	1.00	11.11
7376	C	ARG	B	94	37.673	54.346	57.230	1.00	8.41
7377	O	ARG	B	94	38.537	55.221	57.223	1.00	8.30
7378	N	LEU	B	95	36.655	54.348	58.083	1.00	8.54
7380	CA	LEU	B	95	36.425	55.465	58.999	1.00	8.56
7382	CB	LEU	B	95	35.132	55.266	59.799	1.00	8.44
7385	CG	LEU	B	95	33.814	55.350	59.015	1.00	8.26
7387	CD1	LEU	B	95	32.641	54.912	59.897	1.00	8.69
7391	CD2	LEU	B	95	33.564	56.751	58.449	1.00	7.70
7395	C	LEU	B	95	37.609	55.688	59.938	1.00	8.76
7396	O	LEU	B	95	37.937	56.828	60.249	1.00	8.37
7397	N	MSE	B	96	38.257	54.601	60.363	1.00	9.13
7399	CA	MSE	B	96	39.412	54.671	61.265	1.00	9.46
7401	CB	MSE	B	96	39.512	53.384	62.094	1.00	9.75
7404	CG	MSE	B	96	38.376	53.196	63.075	1.00	11.12
7407	SE	MSE	B	96	38.299	54.659	64.353	1.00	14.97
7408	CE	MSE	B	96	36.822	55.632	63.579	1.00	13.42
7412	C	MSE	B	96	40.744	54.909	60.534	1.00	9.47
7413	O	MSE	B	96	41.792	54.993	61.170	1.00	9.50
7414	N	GLY	B	97	40.705	54.993	59.208	1.00	9.45
7416	CA	GLY	B	97	41.880	55.292	58.406	1.00	9.56
7419	C	GLY	B	97	42.985	54.260	58.558	1.00	9.64
7420	O	GLY	B	97	44.164	54.601	58.532	1.00	9.32
7421	N	ILE	B	98	42.603	52.998	58.728	1.00	9.83
7423	CA	ILE	B	98	43.573	51.917	58.889	1.00	10.10
7425	CB	ILE	B	98	42.876	50.652	59.483	1.00	10.24
7427	CG1	ILE	B	98	42.530	50.906	60.955	1.00	11.02
7430	CD1	ILE	B	98	41.459	50.005	61.506	1.00	12.13
7434	CG2	ILE	B	98	43.757	49.405	59.357	1.00	10.28
7438	C	ILE	B	98	44.244	51.648	57.540	1.00	9.95
7439	O	ILE	B	98	43.622	51.809	56.491	1.00	9.62
7440	N	GLN	B	99	45.520	51.266	57.579	1.00	9.89
7442	CA	GLN	B	99	46.296	51.007	56.368	1.00	9.77
7444	CB	GLN	B	99	47.745	50.621	56.715	1.00	9.84
7447	CG	GLN	B	99	47.909	49.322	57.513	1.00	8.98
7450	CD	GLN	B	99	47.972	48.074	56.646	1.00	8.98
7451	OE1	GLN	B	99	48.396	48.128	55.493	1.00	7.76
7452	NE2	GLN	B	99	47.544	46.945	57.204	1.00	7.65
7455	C	GLN	B	99	45.623	49.925	55.516	1.00	9.97
7456	O	GLN	B	99	44.970	49.026	56.053	1.00	9.88
7457	N	PRO	B	100	45.773	50.016	54.195	1.00	10.26
7458	CA	PRO	B	100	44.968	49.207	53.269	1.00	10.30
7460	CB	PRO	B	100	45.339	49.768	51.888	1.00	10.35

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7463	CG	PRO	B	100	46.666	50.418	52.061	1.00	10.88
7466	CD	PRO	B	100	46.716	50.899	53.482	1.00	10.51
7469	C	PRO	B	100	45.210	47.695	53.310	1.00	10.33
7470	O	PRO	B	100	44.263	46.954	53.071	1.00	10.56
7471	N	PHE	B	101	46.432	47.250	53.581	1.00	10.02
7473	CA	PHE	B	101	46.763	45.828	53.496	1.00	10.15
7475	CB	PHE	B	101	48.242	45.634	53.143	1.00	10.26
7478	CG	PHE	B	101	48.622	46.221	51.805	1.00	11.29
7479	CD1	PHE	B	101	49.511	47.285	51.720	1.00	12.63
7481	CE1	PHE	B	101	49.857	47.834	50.477	1.00	12.90
7483	CZ	PHE	B	101	49.305	47.320	49.316	1.00	13.04
7485	CE2	PHE	B	101	48.413	46.260	49.387	1.00	12.62
7487	CD2	PHE	B	101	48.074	45.718	50.629	1.00	12.53
7489	C	PHE	B	101	46.369	45.073	54.770	1.00	9.98
7490	O	PHE	B	101	47.212	44.663	55.567	1.00	9.84
7491	N	ALA	B	102	45.059	44.911	54.928	1.00	9.66
7493	CA	ALA	B	102	44.451	44.293	56.094	1.00	9.85
7495	CB	ALA	B	102	44.036	45.361	57.088	1.00	9.95
7499	C	ALA	B	102	43.229	43.487	55.667	1.00	9.77
7500	O	ALA	B	102	42.588	43.815	54.666	1.00	9.43
7501	N	ARG	B	103	42.907	42.437	56.421	1.00	9.85
7503	CA	ARG	B	103	41.651	41.725	56.218	1.00	9.82
7505	CB	ARG	B	103	41.834	40.207	56.295	1.00	10.02
7508	CG	ARG	B	103	42.108	39.629	57.661	1.00	10.75
7511	CD	ARG	B	103	42.048	38.113	57.678	1.00	12.03
7514	NE	ARG	B	103	43.157	37.487	56.955	1.00	11.32
7516	CZ	ARG	B	103	44.288	37.050	57.512	1.00	12.65
7517	NH1	ARG	B	103	44.513	37.182	58.815	1.00	13.47
7520	NH2	ARG	B	103	45.219	36.485	56.754	1.00	11.84
7523	C	ARG	B	103	40.615	42.216	57.218	1.00	9.66
7524	O	ARG	B	103	40.935	42.489	58.377	1.00	9.72
7525	N	SER	B	104	39.378	42.338	56.750	1.00	9.01
7527	CA	SER	B	104	38.287	42.864	57.557	1.00	8.81
7529	CB	SER	B	104	37.948	44.297	57.132	1.00	8.73
7532	OG	SER	B	104	39.081	45.146	57.238	1.00	8.12
7534	C	SER	B	104	37.067	41.965	57.411	1.00	8.56
7535	O	SER	B	104	36.683	41.601	56.299	1.00	8.59
7536	N	PHE	B	105	36.478	41.582	58.536	1.00	8.30
7538	CA	PHE	B	105	35.272	40.761	58.516	1.00	8.28
7540	CB	PHE	B	105	35.610	39.294	58.225	1.00	8.17
7543	CG	PHE	B	105	36.596	38.695	59.183	1.00	8.22
7544	CD1	PHE	B	105	37.960	38.767	58.925	1.00	8.53
7546	CE1	PHE	B	105	38.876	38.214	59.803	1.00	9.11
7548	CZ	PHE	B	105	38.435	37.577	60.953	1.00	8.87
7550	CE2	PHE	B	105	37.079	37.502	61.223	1.00	8.82
7552	CD2	PHE	B	105	36.165	38.060	60.340	1.00	8.70
7554	C	PHE	B	105	34.482	40.857	59.806	1.00	8.33
7555	O	PHE	B	105	34.955	41.379	60.815	1.00	8.29
7556	N	GLU	B	106	33.270	40.322	59.732	1.00	8.40
7558	CA	GLU	B	106	32.288	40.335	60.796	1.00	8.41
7560	CB	GLU	B	106	30.952	40.773	60.183	1.00	8.56
7563	CG	GLU	B	106	29.839	41.160	61.133	1.00	8.46

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7566	CD	GLU	B	106	28.616	41.666	60.388	1.00	7.62
7567	OE1	GLU	B	106	27.572	40.981	60.424	1.00	6.66
7568	OE2	GLU	B	106	28.701	42.742	59.749	1.00	6.42
7569	C	GLU	B	106	32.191	38.911	61.333	1.00	8.49
7570	O	GLU	B	106	32.226	37.953	60.550	1.00	8.68
7571	N	ILE	B	107	32.107	38.767	62.656	1.00	8.33
7573	CA	ILE	B	107	31.844	37.479	63.288	1.00	8.42
7575	CB	ILE	B	107	32.900	37.153	64.365	1.00	8.22
7577	CG1	ILE	B	107	34.269	36.975	63.711	1.00	8.66
7580	CD1	ILE	B	107	35.397	36.642	64.670	1.00	8.64
7584	CG2	ILE	B	107	32.503	35.887	65.135	1.00	8.53
7588	C	ILE	B	107	30.452	37.493	63.905	1.00	8.27
7589	O	ILE	B	107	30.074	38.452	64.586	1.00	7.94
7590	N	LYS	B	108	29.702	36.421	63.669	1.00	8.10
7592	CA	LYS	B	108	28.368	36.267	64.222	1.00	8.22
7594	CB	LYS	B	108	27.325	36.269	63.110	1.00	8.28
7597	CG	LYS	B	108	25.881	36.111	63.596	1.00	8.67
7600	CD	LYS	B	108	24.973	35.558	62.499	1.00	9.61
7603	CE	LYS	B	108	24.857	36.503	61.322	1.00	9.93
7606	NZ	LYS	B	108	24.135	35.872	60.183	1.00	10.41
7610	C	LYS	B	108	28.251	34.971	65.009	1.00	8.13
7611	O	LYS	B	108	28.425	33.883	64.464	1.00	8.15
7612	N	GLU	B	109	27.973	35.116	66.298	1.00	8.03
7614	CA	GLU	B	109	27.443	34.045	67.127	1.00	8.05
7616	CB	GLU	B	109	28.492	32.964	67.406	1.00	8.00
7619	CG	GLU	B	109	28.143	31.898	68.448	1.00	8.09
7622	CD	GLU	B	109	26.661	31.724	68.729	1.00	8.51
7623	OE1	GLU	B	109	26.301	31.645	69.920	1.00	9.51
7624	OE2	GLU	B	109	25.861	31.644	67.779	1.00	7.95
7625	C	GLU	B	109	26.956	34.716	68.401	1.00	8.06
7626	O	GLU	B	109	27.618	34.676	69.434	1.00	7.89
7627	N	ALA	B	110	25.820	35.396	68.279	1.00	8.12
7629	CA	ALA	B	110	25.128	35.979	69.412	1.00	8.29
7631	CB	ALA	B	110	24.523	34.858	70.277	1.00	8.28
7635	C	ALA	B	110	26.076	36.889	70.209	1.00	8.41
7636	O	ALA	B	110	26.827	37.666	69.617	1.00	8.54
7637	N	CYS	B	111	26.063	36.785	71.534	1.00	8.54
7639	CA	CYS	B	111	26.910	37.626	72.382	1.00	8.88
7641	CB	CYS	B	111	26.256	37.794	73.745	1.00	8.84
7644	SG	CYS	B	111	24.812	38.846	73.647	1.00	11.06
7645	C	CYS	B	111	28.335	37.104	72.555	1.00	8.69
7646	O	CYS	B	111	29.104	37.654	73.345	1.00	8.74
7647	N	TYR	B	112	28.678	36.056	71.807	1.00	8.59
7649	CA	TYR	B	112	30.005	35.449	71.825	1.00	8.67
7651	CB	TYR	B	112	29.871	33.915	71.746	1.00	8.58
7654	CG	TYR	B	112	31.196	33.209	71.649	1.00	9.19
7655	CD1	TYR	B	112	31.666	32.726	70.427	1.00	9.60
7657	CE1	TYR	B	112	32.898	32.095	70.335	1.00	10.32
7659	CZ	TYR	B	112	33.672	31.958	71.465	1.00	10.38
7660	OH	TYR	B	112	34.889	31.349	71.387	1.00	12.93
7662	CE2	TYR	B	112	33.232	32.439	72.682	1.00	10.52
7664	CD2	TYR	B	112	32.003	33.062	72.766	1.00	9.66

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7666	C	TYR	B	112	30.930	35.963	70.707	1.00	8.60
7667	O	TYR	B	112	32.141	35.782	70.783	1.00	8.62
7668	N	GLY	B	113	30.372	36.636	69.701	1.00	8.82
7670	CA	GLY	B	113	31.113	37.018	68.505	1.00	8.74
7673	C	GLY	B	113	32.401	37.811	68.684	1.00	8.96
7674	O	GLY	B	113	33.387	37.552	67.991	1.00	8.72
7675	N	ALA	B	114	32.398	38.796	69.577	1.00	8.93
7677	CA	ALA	B	114	33.611	39.585	69.832	1.00	8.87
7679	CB	ALA	B	114	33.285	40.851	70.598	1.00	8.96
7683	C	ALA	B	114	34.680	38.776	70.569	1.00	8.89
7684	O	ALA	B	114	35.869	38.987	70.352	1.00	8.80
7685	N	THR	B	115	34.256	37.862	71.441	1.00	8.83
7687	CA	THR	B	115	35.175	36.944	72.111	1.00	8.79
7689	CB	THR	B	115	34.432	36.058	73.133	1.00	8.81
7691	OG1	THR	B	115	33.857	36.874	74.163	1.00	8.88
7693	CG2	THR	B	115	35.407	35.143	73.879	1.00	8.57
7697	C	THR	B	115	35.907	36.059	71.108	1.00	8.94
7698	O	THR	B	115	37.111	35.855	71.232	1.00	9.11
7699	N	ALA	B	116	35.179	35.527	70.130	1.00	9.08
7701	CA	ALA	B	116	35.782	34.768	69.035	1.00	9.15
7703	CB	ALA	B	116	34.716	34.345	68.036	1.00	9.32
7707	C	ALA	B	116	36.852	35.610	68.343	1.00	9.11
7708	O	ALA	B	116	37.966	35.144	68.117	1.00	8.61
7709	N	GLY	B	117	36.500	36.854	68.024	1.00	9.01
7711	CA	GLY	B	117	37.431	37.818	67.464	1.00	9.22
7714	C	GLY	B	117	38.663	38.047	68.325	1.00	9.47
7715	O	GLY	B	117	39.777	38.102	67.809	1.00	9.25
7716	N	LEU	B	118	38.471	38.168	69.637	1.00	9.82
7718	CA	LEU	B	118	39.585	38.410	70.560	1.00	10.30
7720	CB	LEU	B	118	39.072	38.638	71.987	1.00	10.13
7723	CG	LEU	B	118	40.123	38.803	73.095	1.00	10.25
7725	CD1	LEU	B	118	41.049	39.983	72.811	1.00	9.79
7729	CD2	LEU	B	118	39.441	38.970	74.444	1.00	10.10
7733	C	LEU	B	118	40.586	37.249	70.544	1.00	10.80
7734	O	LEU	B	118	41.793	37.473	70.486	1.00	10.33
7735	N	GLN	B	119	40.078	36.019	70.581	1.00	11.80
7737	CA	GLN	B	119	40.937	34.833	70.635	1.00	12.63
7739	CB	GLN	B	119	40.147	33.564	70.998	1.00	12.89
7742	CG	GLN	B	119	39.185	33.659	72.193	1.00	14.42
7745	CD	GLN	B	119	39.807	34.168	73.483	1.00	16.62
7746	OE1	GLN	B	119	40.944	34.635	73.503	1.00	19.22
7747	NE2	GLN	B	119	39.054	34.067	74.574	1.00	18.23
7750	C	GLN	B	119	41.658	34.613	69.312	1.00	12.81
7751	O	GLN	B	119	42.818	34.213	69.298	1.00	13.12
7752	N	LEU	B	120	40.969	34.864	68.204	1.00	13.02
7754	CA	LEU	B	120	41.572	34.728	66.884	1.00	13.42
7756	CB	LEU	B	120	40.523	34.870	65.780	1.00	13.74
7759	CG	LEU	B	120	39.333	33.903	65.756	1.00	15.83
7761	CD1	LEU	B	120	39.710	32.527	65.253	1.00	17.40
7765	CD2	LEU	B	120	38.212	34.496	64.907	1.00	17.31
7769	C	LEU	B	120	42.639	35.804	66.703	1.00	12.90
7770	O	LEU	B	120	43.673	35.559	66.088	1.00	12.94

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7771	N	ALA	B	121	42.372	36.993	67.239	1.00	12.34
7773	CA	ALA	B	121	43.309	38.111	67.168	1.00	12.05
7775	CB	ALA	B	121	42.672	39.383	67.718	1.00	11.75
7779	C	ALA	B	121	44.574	37.770	67.945	1.00	12.04
7780	O	ALA	B	121	45.682	38.039	67.490	1.00	11.38
7781	N	LYS	B	122	44.389	37.159	69.111	1.00	12.10
7783	CA	LYS	B	122	45.493	36.725	69.959	1.00	12.49
7785	CB	LYS	B	122	44.941	36.030	71.215	1.00	12.72
7788	CG	LYS	B	122	45.986	35.456	72.165	1.00	14.03
7791	CD	LYS	B	122	45.341	34.606	73.267	1.00	15.97
7794	CE	LYS	B	122	44.654	33.353	72.721	1.00	17.50
7797	NZ	LYS	B	122	44.366	32.349	73.795	1.00	19.15
7801	C	LYS	B	122	46.434	35.794	69.191	1.00	12.39
7802	O	LYS	B	122	47.650	35.985	69.223	1.00	12.34
7803	N	ASN	B	123	45.872	34.805	68.497	1.00	12.25
7805	CA	ASN	B	123	46.668	33.841	67.732	1.00	12.44
7807	CB	ASN	B	123	45.787	32.725	67.150	1.00	12.60
7810	CG	ASN	B	123	45.086	31.887	68.205	1.00	13.06
7811	OD1	ASN	B	123	44.120	31.198	67.894	1.00	14.34
7812	ND2	ASN	B	123	45.565	31.932	69.442	1.00	13.08
7815	C	ASN	B	123	47.417	34.506	66.572	1.00	12.48
7816	O	ASN	B	123	48.557	34.140	66.264	1.00	12.27
7817	N	HIS	B	124	46.758	35.471	65.928	1.00	12.26
7819	CA	HIS	B	124	47.327	36.198	64.804	1.00	12.30
7821	CB	HIS	B	124	46.276	37.135	64.170	1.00	12.36
7824	CG	HIS	B	124	46.834	38.055	63.126	1.00	12.26
7825	ND1	HIS	B	124	47.222	37.619	61.878	1.00	12.36
7827	CE1	HIS	B	124	47.682	38.641	61.179	1.00	12.09
7829	NE2	HIS	B	124	47.595	39.728	61.925	1.00	12.22
7831	CD2	HIS	B	124	47.071	39.388	63.148	1.00	12.11
7833	C	HIS	B	124	48.558	36.984	65.258	1.00	12.58
7834	O	HIS	B	124	49.609	36.919	64.616	1.00	12.12
7835	N	VAL	B	125	48.431	37.701	66.375	1.00	12.77
7837	CA	VAL	B	125	49.540	38.490	66.912	1.00	13.43
7839	CB	VAL	B	125	49.072	39.485	68.005	1.00	13.44
7841	CG1	VAL	B	125	50.270	40.245	68.598	1.00	13.41
7845	CG2	VAL	B	125	48.049	40.479	67.435	1.00	12.56
7849	C	VAL	B	125	50.664	37.585	67.447	1.00	14.14
7850	O	VAL	B	125	51.837	37.950	67.389	1.00	14.26
7851	N	ALA	B	126	50.313	36.400	67.937	1.00	14.90
7853	CA	ALA	B	126	51.312	35.424	68.381	1.00	15.70
7855	CB	ALA	B	126	50.633	34.190	68.985	1.00	15.74
7859	C	ALA	B	126	52.245	35.009	67.247	1.00	16.23
7860	O	ALA	B	126	53.449	34.860	67.455	1.00	16.73
7861	N	LEU	B	127	51.685	34.839	66.052	1.00	16.80
7863	CA	LEU	B	127	52.455	34.424	64.880	1.00	17.31
7865	CB	LEU	B	127	51.575	33.608	63.918	1.00	17.53
7868	CG	LEU	B	127	51.382	32.088	64.114	1.00	18.75
7870	CD1	LEU	B	127	52.421	31.431	65.039	1.00	19.77
7874	CD2	LEU	B	127	49.984	31.765	64.603	1.00	19.36
7878	C	LEU	B	127	53.066	35.620	64.138	1.00	17.22
7879	O	LEU	B	127	53.945	35.439	63.299	1.00	17.45

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7880	N	HIS	B	128	52.589	36.829	64.441	1.00	17.01
7882	CA	HIS	B	128	53.073	38.065	63.820	1.00	16.68
7884	CB	HIS	B	128	52.142	38.500	62.677	1.00	16.85
7887	CG	HIS	B	128	51.862	37.431	61.663	1.00	17.36
7888	ND1	HIS	B	128	52.743	37.113	60.651	1.00	17.93
7890	CE1	HIS	B	128	52.230	36.146	59.912	1.00	18.58
7892	NE2	HIS	B	128	51.044	35.831	60.402	1.00	17.74
7894	CD2	HIS	B	128	50.789	36.622	61.495	1.00	17.62
7896	C	HIS	B	128	53.128	39.170	64.886	1.00	16.40
7897	O	HIS	B	128	52.307	40.085	64.874	1.00	16.07
7898	N	PRO	B	129	54.086	39.085	65.811	1.00	16.20
7899	CA	PRO	B	129	54.069	39.916	67.025	1.00	16.09
7901	CB	PRO	B	129	55.163	39.286	67.900	1.00	16.24
7904	CG	PRO	B	129	56.065	38.589	66.961	1.00	16.45
7907	CD	PRO	B	129	55.254	38.190	65.770	1.00	16.35
7910	C	PRO	B	129	54.306	41.416	66.827	1.00	15.87
7911	O	PRO	B	129	54.107	42.168	67.782	1.00	15.87
7912	N	ASP	B	130	54.710	41.841	65.633	1.00	15.34
7914	CA	ASP	B	130	54.811	43.270	65.313	1.00	15.42
7916	CB	ASP	B	130	55.965	43.526	64.326	1.00	15.88
7919	CG	ASP	B	130	55.772	42.831	62.980	1.00	17.58
7920	OD1	ASP	B	130	56.308	43.341	61.969	1.00	20.91
7921	OD2	ASP	B	130	55.125	41.769	62.833	1.00	20.55
7922	C	ASP	B	130	53.495	43.884	64.781	1.00	14.64
7923	O	ASP	B	130	53.411	45.093	64.564	1.00	14.32
7924	N	LYS	B	131	52.477	43.054	64.580	1.00	13.73
7926	CA	LYS	B	131	51.191	43.511	64.066	1.00	13.21
7928	CB	LYS	B	131	50.695	42.564	62.968	1.00	13.53
7931	CG	LYS	B	131	51.658	42.392	61.795	1.00	14.63
7934	CD	LYS	B	131	51.913	43.713	61.079	1.00	16.47
7937	CE	LYS	B	131	52.663	43.516	59.780	1.00	18.03
7940	NZ	LYS	B	131	52.937	44.831	59.113	1.00	19.37
7944	C	LYS	B	131	50.147	43.615	65.178	1.00	12.34
7945	O	LYS	B	131	50.301	43.031	66.256	1.00	11.80
7946	N	LYS	B	132	49.083	44.361	64.895	1.00	11.49
7948	CA	LYS	B	132	47.995	44.579	65.842	1.00	11.10
7950	CB	LYS	B	132	48.015	46.020	66.363	1.00	10.95
7953	CG	LYS	B	132	49.374	46.483	66.884	1.00	11.28
7956	CD	LYS	B	132	49.303	47.891	67.471	1.00	11.09
7959	CE	LYS	B	132	50.689	48.501	67.651	1.00	11.33
7962	NZ	LYS	B	132	50.657	49.803	68.384	1.00	11.67
7966	C	LYS	B	132	46.645	44.283	65.188	1.00	10.70
7967	O	LYS	B	132	46.523	44.266	63.965	1.00	10.35
7968	N	VAL	B	133	45.637	44.041	66.018	1.00	10.17
7970	CA	VAL	B	133	44.296	43.746	65.542	1.00	9.79
7972	CB	VAL	B	133	43.926	42.269	65.786	1.00	9.67
7974	CG1	VAL	B	133	42.547	41.952	65.215	1.00	9.58
7978	CG2	VAL	B	133	44.976	41.351	65.183	1.00	9.63
7982	C	VAL	B	133	43.290	44.621	66.269	1.00	9.60
7983	O	VAL	B	133	43.346	44.757	67.487	1.00	9.85
7984	N	LEU	B	134	42.376	45.221	65.515	1.00	9.11
7986	CA	LEU	B	134	41.251	45.934	66.099	1.00	8.74

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7988	CB	LEU	B	134	40.865	47.133	65.232	1.00	8.86
7991	CG	LEU	B	134	39.605	47.893	65.655	1.00	8.70
7993	CD1	LEU	B	134	39.760	48.449	67.060	1.00	9.48
7997	CD2	LEU	B	134	39.303	48.999	64.662	1.00	9.46
8001	C	LEU	B	134	40.078	44.968	66.200	1.00	8.50
8002	O	LEU	B	134	39.638	44.430	65.193	1.00	8.27
8003	N	VAL	B	135	39.595	44.738	67.416	1.00	8.22
8005	CA	VAL	B	135	38.417	43.911	67.652	1.00	8.36
8007	CB	VAL	B	135	38.745	42.703	68.551	1.00	8.37
8009	CG1	VAL	B	135	37.491	41.861	68.818	1.00	8.54
8013	CG2	VAL	B	135	39.856	41.860	67.927	1.00	8.48
8017	C	VAL	B	135	37.359	44.772	68.329	1.00	8.17
8018	O	VAL	B	135	37.590	45.297	69.410	1.00	8.27
8019	N	VAL	B	136	36.198	44.905	67.695	1.00	8.09
8021	CA	VAL	B	136	35.125	45.731	68.222	1.00	7.93
8023	CB	VAL	B	136	34.880	46.973	67.334	1.00	7.88
8025	CG1	VAL	B	136	33.836	47.879	67.967	1.00	8.08
8029	CG2	VAL	B	136	36.183	47.739	67.114	1.00	7.70
8033	C	VAL	B	136	33.827	44.943	68.360	1.00	7.83
8034	O	VAL	B	136	33.331	44.371	67.393	1.00	7.80
8035	N	ALA	B	137	33.319	44.890	69.588	1.00	7.75
8037	CA	ALA	B	137	31.964	44.458	69.882	1.00	7.86
8039	CB	ALA	B	137	31.871	44.001	71.325	1.00	7.93
8043	C	ALA	B	137	31.038	45.649	69.654	1.00	7.97
8044	O	ALA	B	137	31.302	46.732	70.153	1.00	8.11
8045	N	ALA	B	138	29.968	45.449	68.895	1.00	7.73
8047	CA	ALA	B	138	29.015	46.515	68.598	1.00	7.67
8049	CB	ALA	B	138	29.446	47.285	67.359	1.00	7.78
8053	C	ALA	B	138	27.634	45.916	68.400	1.00	7.68
8054	O	ALA	B	138	27.470	44.967	67.641	1.00	7.88
8055	N	ASP	B	139	26.641	46.461	69.095	1.00	7.64
8057	CA	ASP	B	139	25.299	45.890	69.068	1.00	7.54
8059	CB	ASP	B	139	25.247	44.597	69.896	1.00	7.44
8062	CG	ASP	B	139	25.578	43.352	69.082	1.00	7.51
8063	OD1	ASP	B	139	24.936	43.119	68.031	1.00	6.08
8064	OD2	ASP	B	139	26.468	42.547	69.423	1.00	6.25
8065	C	ASP	B	139	24.253	46.860	69.600	1.00	7.50
8066	O	ASP	B	139	24.557	47.804	70.332	1.00	7.14
8067	N	ILE	B	140	23.015	46.606	69.200	1.00	7.60
8069	CA	ILE	B	140	21.848	47.328	69.680	1.00	7.83
8071	CB	ILE	B	140	21.235	48.168	68.543	1.00	7.89
8073	CG1	ILE	B	140	22.179	49.309	68.155	1.00	8.01
8076	CD1	ILE	B	140	22.021	49.766	66.722	1.00	8.36
8080	CG2	ILE	B	140	19.875	48.735	68.950	1.00	8.22
8084	C	ILE	B	140	20.871	46.260	70.153	1.00	7.95
8085	O	ILE	B	140	20.359	45.483	69.346	1.00	7.95
8086	N	ALA	B	141	20.653	46.196	71.462	1.00	8.00
8088	CA	ALA	B	141	19.764	45.194	72.057	1.00	8.17
8090	CB	ALA	B	141	20.332	44.703	73.381	1.00	8.32
8094	C	ALA	B	141	18.356	45.745	72.254	1.00	8.33
8095	O	ALA	B	141	18.084	46.445	73.236	1.00	8.23
8096	N	LYS	B	142	17.478	45.433	71.301	1.00	8.58

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8098	CA	LYS	B	142	16.060	45.803	71.352	1.00	8.81
8100	CB	LYS	B	142	15.728	46.766	70.206	1.00	8.77
8103	CG	LYS	B	142	16.444	48.102	70.284	1.00	8.96
8106	CD	LYS	B	142	16.297	48.917	68.995	1.00	9.53
8109	CE	LYS	B	142	14.880	49.443	68.792	1.00	9.66
8112	NZ	LYS	B	142	14.829	50.591	67.824	1.00	9.14
8116	C	LYS	B	142	15.185	44.554	71.243	1.00	8.84
8117	O	LYS	B	142	15.345	43.766	70.317	1.00	8.63
8118	N	TYR	B	143	14.276	44.383	72.204	1.00	9.18
8120	CA	TYR	B	143	13.365	43.237	72.270	1.00	9.43
8122	CB	TYR	B	143	13.354	42.659	73.688	1.00	9.55
8125	CG	TYR	B	143	14.573	41.839	74.047	1.00	9.30
8126	CD1	TYR	B	143	15.687	42.433	74.639	1.00	9.59
8128	CE1	TYR	B	143	16.808	41.681	74.980	1.00	9.01
8130	CZ	TYR	B	143	16.819	40.318	74.734	1.00	8.66
8131	OH	TYR	B	143	17.925	39.573	75.073	1.00	8.51
8133	CE2	TYR	B	143	15.726	39.704	74.153	1.00	8.87
8135	CD2	TYR	B	143	14.608	40.466	73.812	1.00	8.96
8137	C	TYR	B	143	11.931	43.600	71.884	1.00	9.83
8138	O	TYR	B	143	11.194	42.758	71.365	1.00	10.11
8139	N	GLY	B	144	11.532	44.839	72.170	1.00	10.33
8141	CA	GLY	B	144	10.205	45.333	71.843	1.00	10.47
8144	C	GLY	B	144	9.529	45.982	73.036	1.00	10.78
8145	O	GLY	B	144	9.742	45.570	74.172	1.00	10.58
8146	N	LEU	B	145	8.724	47.007	72.774	1.00	11.32
8148	CA	LEU	B	145	7.933	47.661	73.811	1.00	11.74
8150	CB	LEU	B	145	7.177	48.865	73.238	1.00	11.94
8153	CG	LEU	B	145	8.017	49.960	72.572	1.00	12.14
8155	CD1	LEU	B	145	7.117	51.050	72.011	1.00	12.72
8159	CD2	LEU	B	145	9.033	50.538	73.542	1.00	12.06
8163	C	LEU	B	145	6.941	46.652	74.389	1.00	12.01
8164	O	LEU	B	145	6.276	45.946	73.637	1.00	11.59
8165	N	ASN	B	146	6.863	46.595	75.721	1.00	12.51
8167	CA	ASN	B	146	6.017	45.636	76.452	1.00	12.94
8169	CB	ASN	B	146	4.542	45.831	76.082	1.00	13.33
8172	CG	ASN	B	146	4.098	47.264	76.252	1.00	14.31
8173	OD1	ASN	B	146	3.888	47.987	75.276	1.00	16.27
8174	ND2	ASN	B	146	3.983	47.693	77.499	1.00	16.21
8177	C	ASN	B	146	6.411	44.160	76.318	1.00	13.06
8178	O	ASN	B	146	5.645	43.274	76.699	1.00	13.05
8179	N	SER	B	147	7.616	43.900	75.811	1.00	13.04
8181	CA	SER	B	147	8.113	42.533	75.659	1.00	12.90
8183	CB	SER	B	147	9.121	42.455	74.509	1.00	12.89
8186	OG	SER	B	147	10.333	43.115	74.850	1.00	12.61
8188	C	SER	B	147	8.771	42.071	76.951	1.00	12.53
8189	O	SER	B	147	9.125	42.885	77.800	1.00	12.93
8190	N	GLY	B	148	8.943	40.760	77.090	1.00	12.38
8192	CA	GLY	B	148	9.605	40.188	78.249	1.00	11.89
8195	C	GLY	B	148	11.045	40.655	78.391	1.00	11.37
8196	O	GLY	B	148	11.514	40.909	79.501	1.00	11.34
8197	N	GLY	B	149	11.740	40.789	77.265	1.00	10.90
8199	CA	GLY	B	149	13.153	41.135	77.266	1.00	10.49

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8202	C	GLY	B	149	13.443	42.623	77.388	1.00	10.06
8203	O	GLY	B	149	14.593	43.007	77.601	1.00	9.72
8204	N	GLU	B	150	12.407	43.454	77.263	1.00	9.69
8206	CA	GLU	B	150	12.567	44.918	77.223	1.00	9.53
8208	CB	GLU	B	150	11.204	45.622	77.183	1.00	9.34
8211	CG	GLU	B	150	11.290	47.087	76.783	1.00	9.48
8214	CD	GLU	B	150	10.016	47.863	77.052	1.00	10.62
8215	OE1	GLU	B	150	9.052	47.279	77.590	1.00	10.58
8216	OE2	GLU	B	150	9.986	49.064	76.724	1.00	9.89
8217	C	GLU	B	150	13.413	45.532	78.347	1.00	9.25
8218	O	GLU	B	150	14.248	46.391	78.066	1.00	9.16
8219	N	PRO	B	151	13.194	45.131	79.605	1.00	9.25
8220	CA	PRO	B	151	13.958	45.693	80.730	1.00	9.23
8222	CB	PRO	B	151	13.405	44.937	81.942	1.00	9.45
8225	CG	PRO	B	151	12.075	44.446	81.513	1.00	9.61
8228	CD	PRO	B	151	12.211	44.135	80.066	1.00	8.94
8231	C	PRO	B	151	15.477	45.493	80.649	1.00	9.19
8232	O	PRO	B	151	16.214	46.273	81.261	1.00	9.22
8233	N	THR	B	152	15.921	44.468	79.921	1.00	8.82
8235	CA	THR	B	152	17.344	44.152	79.785	1.00	8.61
8237	CB	THR	B	152	17.555	42.621	79.694	1.00	8.63
8239	OG1	THR	B	152	17.028	42.128	78.453	1.00	8.95
8241	CG2	THR	B	152	16.763	41.886	80.764	1.00	8.67
8245	C	THR	B	152	17.997	44.796	78.567	1.00	8.36
8246	O	THR	B	152	19.147	44.491	78.257	1.00	8.40
8247	N	GLN	B	153	17.276	45.681	77.883	1.00	7.85
8249	CA	GLN	B	153	17.777	46.322	76.666	1.00	7.65
8251	CB	GLN	B	153	16.664	47.139	75.993	1.00	7.68
8254	CG	GLN	B	153	15.611	46.288	75.283	1.00	7.72
8257	CD	GLN	B	153	14.399	47.081	74.788	1.00	7.97
8258	OE1	GLN	B	153	13.551	46.527	74.101	1.00	9.28
8259	NE2	GLN	B	153	14.316	48.364	75.134	1.00	8.06
8262	C	GLN	B	153	18.986	47.222	76.931	1.00	7.38
8263	O	GLN	B	153	19.236	47.641	78.055	1.00	7.46
8264	N	GLY	B	154	19.726	47.507	75.869	1.00	7.38
8266	CA	GLY	B	154	20.889	48.375	75.923	1.00	7.46
8269	C	GLY	B	154	21.444	48.585	74.529	1.00	7.64
8270	O	GLY	B	154	20.883	48.087	73.566	1.00	7.33
8271	N	ALA	B	155	22.549	49.316	74.427	1.00	7.89
8273	CA	ALA	B	155	23.181	49.601	73.140	1.00	7.90
8275	CB	ALA	B	155	22.317	50.560	72.322	1.00	8.10
8279	C	ALA	B	155	24.570	50.204	73.343	1.00	7.98
8280	O	ALA	B	155	24.806	50.918	74.317	1.00	8.15
8281	N	GLY	B	156	25.481	49.917	72.416	1.00	7.63
8283	CA	GLY	B	156	26.831	50.447	72.481	1.00	7.64
8286	C	GLY	B	156	27.875	49.576	71.811	1.00	7.52
8287	O	GLY	B	156	27.554	48.639	71.086	1.00	7.33
8288	N	ALA	B	157	29.138	49.907	72.062	1.00	7.42
8290	CA	ALA	B	157	30.268	49.175	71.507	1.00	7.45
8292	CB	ALA	B	157	30.686	49.783	70.163	1.00	7.48
8296	C	ALA	B	157	31.449	49.174	72.475	1.00	7.41
8297	O	ALA	B	157	31.610	50.089	73.273	1.00	7.56

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8298	N	VAL	B	158	32.252	48.123	72.414	1.00	7.38
8300	CA	VAL	B	158	33.511	48.054	73.139	1.00	7.44
8302	CB	VAL	B	158	33.476	46.939	74.204	1.00	7.44
8304	CG1	VAL	B	158	34.813	46.818	74.919	1.00	7.73
8308	CG2	VAL	B	158	32.357	47.203	75.207	1.00	7.87
8312	C	VAL	B	158	34.615	47.787	72.118	1.00	7.43
8313	O	VAL	B	158	34.581	46.776	71.420	1.00	7.72
8314	N	ALA	B	159	35.576	48.701	72.023	1.00	7.54
8316	CA	ALA	B	159	36.707	48.559	71.112	1.00	7.67
8318	CB	ALA	B	159	36.985	49.877	70.416	1.00	7.65
8322	C	ALA	B	159	37.949	48.082	71.860	1.00	7.94
8323	O	ALA	B	159	38.237	48.548	72.961	1.00	7.80
8324	N	MSE	B	160	38.689	47.163	71.245	1.00	8.28
8326	CA	MSE	B	160	39.903	46.602	71.838	1.00	8.72
8328	CB	MSE	B	160	39.640	45.185	72.359	1.00	8.94
8331	CG	MSE	B	160	38.753	45.121	73.593	1.00	10.14
8334	SE	MSE	B	160	38.329	43.270	74.135	1.00	11.99
8335	CE	MSE	B	160	36.877	42.945	72.912	1.00	11.36
8339	C	MSE	B	160	41.023	46.559	70.811	1.00	8.80
8340	O	MSE	B	160	40.801	46.196	69.658	1.00	8.95
8341	N	LEU	B	161	42.225	46.932	71.230	1.00	8.66
8343	CA	LEU	B	161	43.415	46.767	70.414	1.00	8.46
8345	CB	LEU	B	161	44.276	48.033	70.436	1.00	8.45
8348	CG	LEU	B	161	45.492	48.027	69.504	1.00	8.58
8350	CD1	LEU	B	161	45.073	48.003	68.032	1.00	8.89
8354	CD2	LEU	B	161	46.386	49.231	69.791	1.00	8.77
8358	C	LEU	B	161	44.192	45.591	70.980	1.00	8.40
8359	O	LEU	B	161	44.561	45.598	72.152	1.00	8.28
8360	N	VAL	B	162	44.422	44.585	70.144	1.00	8.18
8362	CA	VAL	B	162	45.144	43.384	70.537	1.00	8.30
8364	CB	VAL	B	162	44.472	42.113	69.978	1.00	8.27
8366	CG1	VAL	B	162	45.188	40.860	70.475	1.00	8.59
8370	CG2	VAL	B	162	42.990	42.076	70.363	1.00	8.38
8374	C	VAL	B	162	46.559	43.511	69.994	1.00	8.38
8375	O	VAL	B	162	46.750	43.809	68.819	1.00	7.75
8376	N	ALA	B	163	47.544	43.302	70.861	1.00	8.59
8378	CA	ALA	B	163	48.946	43.478	70.502	1.00	8.99
8380	CB	ALA	B	163	49.297	44.958	70.504	1.00	9.16
8384	C	ALA	B	163	49.865	42.718	71.452	1.00	9.45
8385	O	ALA	B	163	49.431	42.246	72.505	1.00	9.76
8386	N	SER	B	164	51.131	42.594	71.064	1.00	9.94
8388	CA	SER	B	164	52.172	42.063	71.943	1.00	10.28
8390	CB	CSER	B	164	53.437	41.709	71.150	0.35	10.32
8391	CB	BSER	B	164	53.450	41.741	71.159	0.65	10.38
8396	OG	CSER	B	164	53.903	42.811	70.387	0.35	9.93
8397	OG	BSER	B	164	53.186	40.902	70.050	0.65	10.21
8400	C	SER	B	164	52.493	43.082	73.030	1.00	10.76
8401	O	SER	B	164	52.307	44.287	72.836	1.00	10.77
8402	N	GLU	B	165	52.999	42.585	74.160	1.00	11.20
8404	CA	GLU	B	165	53.299	43.405	75.329	1.00	11.54
8406	CB	GLU	B	165	54.626	44.150	75.115	1.00	12.16
8409	CG	GLU	B	165	55.805	43.232	74.796	1.00	13.93

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8412	CD	GLU	B	165	55.915	42.063	75.765	1.00	17.09
8413	OE1	GLU	B	165	55.936	42.317	76.992	1.00	19.30
8414	OE2	GLU	B	165	55.953	40.894	75.308	1.00	18.56
8415	C	GLU	B	165	52.153	44.369	75.657	1.00	11.24
8416	O	GLU	B	165	52.359	45.583	75.776	1.00	10.79
8417	N	PRO	B	166	50.947	43.822	75.831	1.00	10.89
8418	CA	PRO	B	166	49.754	44.651	76.021	1.00	10.95
8420	CB	PRO	B	166	48.621	43.625	76.077	1.00	10.82
8423	CG	PRO	B	166	49.274	42.380	76.556	1.00	11.03
8426	CD	PRO	B	166	50.626	42.385	75.909	1.00	10.81
8429	C	PRO	B	166	49.837	45.433	77.326	1.00	10.98
8430	O	PRO	B	166	50.400	44.935	78.287	1.00	10.75
8431	N	ARG	B	167	49.281	46.637	77.346	1.00	10.96
8433	CA	ARG	B	167	49.399	47.517	78.499	1.00	11.18
8435	CB	ARG	B	167	49.287	48.987	78.055	1.00	11.45
8438	CG	ARG	B	167	50.581	49.534	77.448	1.00	12.90
8441	CD	ARG	B	167	50.424	50.860	76.698	1.00	14.86
8444	NE	ARG	B	167	50.259	50.666	75.260	1.00	16.79
8446	CZ	ARG	B	167	49.959	51.629	74.382	1.00	16.60
8447	NH1	ARG	B	167	49.795	52.899	74.763	1.00	15.61
8450	NH2	ARG	B	167	49.834	51.313	73.102	1.00	16.08
8453	C	ARG	B	167	48.387	47.212	79.614	1.00	10.98
8454	O	ARG	B	167	48.569	47.691	80.732	1.00	10.91
8455	N	ILE	B	168	47.350	46.415	79.326	1.00	10.68
8457	CA	ILE	B	168	46.294	46.132	80.311	1.00	10.64
8459	CB	ILE	B	168	44.918	46.639	79.812	1.00	10.76
8461	CG1	ILE	B	168	44.967	48.153	79.587	1.00	11.06
8464	CD1	ILE	B	168	43.772	48.700	78.863	1.00	12.01
8468	CG2	ILE	B	168	43.821	46.294	80.822	1.00	10.75
8472	C	ILE	B	168	46.196	44.660	80.725	1.00	10.54
8473	O	ILE	B	168	46.397	44.339	81.893	1.00	10.43
8474	N	LEU	B	169	45.879	43.776	79.781	1.00	10.23
8476	CA	LEU	B	169	45.569	42.387	80.114	1.00	10.23
8478	CB	LEU	B	169	44.049	42.171	80.091	1.00	9.99
8481	CG	LEU	B	169	43.525	40.930	80.825	1.00	9.91
8483	CD1	LEU	B	169	43.568	41.129	82.329	1.00	9.70
8487	CD2	LEU	B	169	42.111	40.586	80.373	1.00	9.88
8491	C	LEU	B	169	46.267	41.388	79.188	1.00	10.33
8492	O	LEU	B	169	45.963	41.317	78.000	1.00	10.25
8493	N	ALA	B	170	47.212	40.631	79.745	1.00	10.57
8495	CA	ALA	B	170	47.868	39.536	79.033	1.00	10.87
8497	CB	ALA	B	170	49.232	39.250	79.647	1.00	10.89
8501	C	ALA	B	170	47.001	38.282	79.088	1.00	11.28
8502	O	ALA	B	170	46.656	37.815	80.167	1.00	11.30
8503	N	LEU	B	171	46.661	37.732	77.929	1.00	11.66
8505	CA	LEU	B	171	45.806	36.551	77.859	1.00	12.24
8507	CB	LEU	B	171	45.013	36.558	76.549	1.00	12.25
8510	CG	LEU	B	171	44.106	37.782	76.348	1.00	11.63
8512	CD1	LEU	B	171	43.544	37.831	74.935	1.00	11.53
8516	CD2	LEU	B	171	42.976	37.799	77.376	1.00	11.69
8520	C	LEU	B	171	46.624	35.255	77.989	1.00	13.05
8521	O	LEU	B	171	47.708	35.132	77.419	1.00	12.95

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8522	N	LYS	B	172	46.085	34.306	78.750	1.00	13.99
8524	CA	LYS	B	172	46.695	32.995	78.964	1.00	15.08
8526	CB	LYS	B	172	46.414	32.507	80.390	1.00	15.29
8529	CG	LYS	B	172	46.804	33.482	81.491	1.00	16.94
8532	CD	LYS	B	172	48.292	33.424	81.797	1.00	19.62
8535	CE	LYS	B	172	48.628	34.075	83.138	1.00	20.83
8538	NZ	LYS	B	172	48.827	33.064	84.226	1.00	22.61
8542	C	LYS	B	172	46.119	31.992	77.964	1.00	15.35
8543	O	LYS	B	172	45.169	32.308	77.247	1.00	15.43
8544	N	GLU	B	173	46.689	30.788	77.932	1.00	15.73
8546	CA	GLU	B	173	46.270	29.738	76.996	1.00	16.26
8548	CB	GLU	B	173	47.486	29.150	76.266	1.00	16.67
8551	CG	GLU	B	173	48.240	30.136	75.385	1.00	18.61
8554	CD	GLU	B	173	47.443	30.585	74.169	1.00	21.34
8555	OE1	GLU	B	173	47.262	29.774	73.234	1.00	23.06
8556	OE2	GLU	B	173	47.003	31.756	74.138	1.00	23.86
8557	C	GLU	B	173	45.520	28.621	77.724	1.00	15.94
8558	O	GLU	B	173	45.843	27.440	77.574	1.00	16.49
8559	N	ASP	B	174	44.513	29.002	78.500	1.00	15.24
8561	CA	ASP	B	174	43.759	28.057	79.322	1.00	14.89
8563	CB	ASP	B	174	43.894	28.427	80.811	1.00	14.66
8566	CG	ASP	B	174	43.178	29.725	81.175	1.00	14.76
8567	OD1	ASP	B	174	43.044	30.622	80.303	1.00	13.61
8568	OD2	ASP	B	174	42.717	29.931	82.321	1.00	13.29
8569	C	ASP	B	174	42.289	27.996	78.893	1.00	14.59
8570	O	ASP	B	174	41.416	27.633	79.682	1.00	14.62
8571	N	ASN	B	175	42.040	28.316	77.623	1.00	14.44
8573	CA	ASN	B	175	40.680	28.481	77.100	1.00	14.16
8575	CB	ASN	B	175	40.701	28.987	75.646	1.00	14.33
8578	CG	ASN	B	175	41.486	30.294	75.475	1.00	15.12
8579	OD1	ASN	B	175	42.713	30.322	75.635	1.00	16.74
8580	ND2	ASN	B	175	40.782	31.375	75.137	1.00	14.01
8583	C	ASN	B	175	39.910	27.164	77.155	1.00	13.87
8584	O	ASN	B	175	40.426	26.124	76.744	1.00	13.49
8585	N	VAL	B	176	38.692	27.217	77.692	1.00	13.21
8587	CA	VAL	B	176	37.743	26.118	77.617	1.00	12.91
8589	CB	VAL	B	176	37.371	25.559	78.999	1.00	13.03
8591	CG1	VAL	B	176	36.224	24.543	78.877	1.00	13.31
8595	CG2	VAL	B	176	38.580	24.931	79.657	1.00	13.59
8599	C	VAL	B	176	36.481	26.637	76.959	1.00	12.50
8600	O	VAL	B	176	35.832	27.546	77.467	1.00	12.27
8601	N	MET	B	177	36.127	26.033	75.837	1.00	12.05
8603	CA	MET	B	177	34.972	26.462	75.061	1.00	11.83
8605	CB	MET	B	177	35.411	26.923	73.677	1.00	11.77
8608	CG	MET	B	177	36.527	26.103	73.097	1.00	11.89
8611	SD	MET	B	177	38.183	26.790	73.399	1.00	8.57
8612	CE	MET	B	177	38.703	26.682	71.741	1.00	10.96
8616	C	MET	B	177	33.956	25.329	74.962	1.00	11.70
8617	O	MET	B	177	34.264	24.175	75.256	1.00	11.25
8618	N	LEU	B	178	32.748	25.678	74.534	1.00	11.42
8620	CA	LEU	B	178	31.619	24.765	74.547	1.00	11.25
8622	CB	LEU	B	178	30.981	24.756	75.939	1.00	11.37

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8625	CG	LEU	B	178	29.700	23.939	76.129	1.00	12.09
8627	CD1	LEU	B	178	29.983	22.459	75.939	1.00	12.70
8631	CD2	LEU	B	178	29.091	24.203	77.499	1.00	12.56
8635	C	LEU	B	178	30.590	25.197	73.504	1.00	10.91
8636	O	LEU	B	178	30.248	26.368	73.419	1.00	10.41
8637	N	THR	B	179	30.111	24.240	72.715	1.00	10.56
8639	CA	THR	B	179	29.021	24.461	71.770	1.00	10.66
8641	CB	THR	B	179	29.521	24.294	70.315	1.00	10.50
8643	OG1	THR	B	179	30.467	25.322	69.994	1.00	10.71
8645	CG2	THR	B	179	28.385	24.506	69.323	1.00	10.71
8649	C	THR	B	179	27.911	23.445	72.034	1.00	10.76
8650	O	THR	B	179	28.168	22.247	72.078	1.00	10.27
8651	N	GLN	B	180	26.689	23.936	72.217	1.00	11.16
8653	CA	GLN	B	180	25.488	23.103	72.284	1.00	11.76
8655	CB	GLN	B	180	24.957	23.018	73.711	1.00	11.95
8658	CG	GLN	B	180	25.932	22.527	74.745	1.00	13.46
8661	CD	GLN	B	180	25.410	22.765	76.145	1.00	15.16
8662	OE1	GLN	B	180	25.704	23.793	76.752	1.00	17.63
8663	NE2	GLN	B	180	24.614	21.831	76.650	1.00	16.39
8666	C	GLN	B	180	24.408	23.745	71.432	1.00	11.70
8667	O	GLN	B	180	24.218	24.947	71.502	1.00	12.41
8668	N	ASP	B	181	23.680	22.950	70.660	1.00	11.52
8670	CA	ASP	B	181	22.600	23.464	69.824	1.00	11.31
8672	CB	ASP	B	181	22.404	22.543	68.622	1.00	11.40
8675	CG	ASP	B	181	21.445	23.106	67.594	1.00	11.56
8676	OD1	ASP	B	181	20.798	24.147	67.853	1.00	10.88
8677	OD2	ASP	B	181	21.280	22.555	66.487	1.00	12.11
8678	C	ASP	B	181	21.308	23.583	70.635	1.00	11.19
8679	O	ASP	B	181	20.555	22.616	70.778	1.00	10.91
8680	N	ILE	B	182	21.076	24.779	71.174	1.00	10.93
8682	CA	ILE	B	182	19.920	25.074	72.016	1.00	10.73
8684	CB	ILE	B	182	20.363	25.193	73.489	1.00	10.94
8686	CG1	ILE	B	182	20.862	23.844	74.021	1.00	11.42
8689	CD1	ILE	B	182	21.734	23.973	75.259	1.00	12.34
8693	CG2	ILE	B	182	19.220	25.719	74.364	1.00	11.11
8697	C	ILE	B	182	19.275	26.392	71.582	1.00	10.45
8698	O	ILE	B	182	19.967	27.407	71.442	1.00	10.34
8699	N	TYR	B	183	17.955	26.379	71.408	1.00	9.81
8701	CA	TYR	B	183	17.212	27.562	70.964	1.00	9.51
8703	CB	TYR	B	183	16.141	27.172	69.938	1.00	9.43
8706	CG	TYR	B	183	16.708	27.045	68.539	1.00	8.81
8707	CD1	TYR	B	183	16.838	28.159	67.723	1.00	7.75
8709	CE1	TYR	B	183	17.367	28.060	66.441	1.00	7.71
8711	CZ	TYR	B	183	17.784	26.833	65.966	1.00	7.80
8712	OH	TYR	B	183	18.310	26.745	64.697	1.00	7.51
8714	CE2	TYR	B	183	17.671	25.703	66.759	1.00	8.21
8716	CD2	TYR	B	183	17.137	25.813	68.042	1.00	8.40
8718	C	TYR	B	183	16.633	28.349	72.144	1.00	9.13
8719	O	TYR	B	183	15.418	28.438	72.338	1.00	8.73
8720	N	ASP	B	184	17.539	28.928	72.924	1.00	8.82
8722	CA	ASP	B	184	17.172	29.790	74.041	1.00	8.64
8724	CB	ASP	B	184	18.255	29.771	75.131	1.00	8.83

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8727	CG	ASP	B	184	19.589	30.358	74.671	1.00	8.74
8728	OD1	ASP	B	184	20.207	31.130	75.445	1.00	9.11
8729	OD2	ASP	B	184	20.107	30.097	73.565	1.00	7.83
8730	C	ASP	B	184	16.881	31.216	73.567	1.00	8.74
8731	O	ASP	B	184	15.977	31.883	74.077	1.00	8.78
8732	N	PHE	B	185	17.647	31.664	72.581	1.00	8.37
8734	CA	PHE	B	185	17.526	33.006	72.025	1.00	8.42
8736	CB	PHE	B	185	18.216	34.025	72.954	1.00	8.49
8739	CG	PHE	B	185	18.548	35.370	72.324	1.00	8.38
8740	CD1	PHE	B	185	18.014	36.540	72.858	1.00	8.75
8742	CE1	PHE	B	185	18.327	37.785	72.317	1.00	8.58
8744	CZ	PHE	B	185	19.202	37.875	71.243	1.00	8.36
8746	CE2	PHE	B	185	19.751	36.727	70.712	1.00	7.46
8748	CD2	PHE	B	185	19.440	35.482	71.262	1.00	7.98
8750	C	PHE	B	185	18.131	32.944	70.627	1.00	8.34
8751	O	PHE	B	185	19.178	32.325	70.407	1.00	8.33
8752	N	TRP	B	186	17.432	33.550	69.682	1.00	8.38
8754	CA	TRP	B	186	17.865	33.602	68.297	1.00	8.40
8756	CB	TRP	B	186	17.690	32.235	67.623	1.00	8.43
8759	CG	TRP	B	186	16.263	31.801	67.389	1.00	8.00
8760	CD1	TRP	B	186	15.629	31.740	66.191	1.00	8.14
8762	NE1	TRP	B	186	14.345	31.279	66.350	1.00	7.86
8764	CE2	TRP	B	186	14.126	31.020	67.676	1.00	7.75
8765	CD2	TRP	B	186	15.316	31.331	68.364	1.00	7.70
8766	CE3	TRP	B	186	15.348	31.147	69.755	1.00	7.21
8768	CZ3	TRP	B	186	14.207	30.683	70.396	1.00	7.64
8770	CH2	TRP	B	186	13.045	30.380	69.678	1.00	7.63
8772	CZ2	TRP	B	186	12.982	30.547	68.322	1.00	7.78
8774	C	TRP	B	186	17.067	34.691	67.589	1.00	8.47
8775	O	TRP	B	186	16.179	35.286	68.179	1.00	8.45
8776	N	ARG	B	187	17.404	34.985	66.342	1.00	8.48
8778	CA	ARG	B	187	16.679	36.006	65.591	1.00	8.58
8780	CB	ARG	B	187	17.307	37.390	65.792	1.00	8.52
8783	CG	ARG	B	187	16.472	38.518	65.199	1.00	8.34
8786	CD	ARG	B	187	16.677	39.869	65.858	1.00	8.54
8789	NE	ARG	B	187	17.964	40.470	65.516	1.00	7.93
8791	CZ	ARG	B	187	18.245	41.054	64.352	1.00	9.02
8792	NH1	ARG	B	187	17.339	41.136	63.393	1.00	9.12
8795	NH2	ARG	B	187	19.446	41.577	64.149	1.00	8.63
8798	C	ARG	B	187	16.633	35.646	64.113	1.00	8.78
8799	O	ARG	B	187	17.540	35.993	63.366	1.00	8.58
8800	N	PRO	B	188	15.573	34.957	63.688	1.00	9.19
8801	CA	PRO	B	188	15.460	34.522	62.294	1.00	9.40
8803	CB	PRO	B	188	14.075	33.862	62.230	1.00	9.46
8806	CG	PRO	B	188	13.726	33.526	63.625	1.00	9.61
8809	CD	PRO	B	188	14.397	34.562	64.486	1.00	9.35
8812	C	PRO	B	188	15.524	35.704	61.341	1.00	9.56
8813	O	PRO	B	188	15.115	36.810	61.704	1.00	9.65
8814	N	THR	B	189	16.036	35.465	60.140	1.00	9.76
8816	CA	THR	B	189	16.058	36.476	59.087	1.00	9.94
8818	CB	THR	B	189	16.457	35.830	57.744	1.00	9.93
8820	OG1	THR	B	189	17.705	35.144	57.886	1.00	10.67

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8822	CG2	THR	B	189	16.741	36.885	56.686	1.00	10.40
8826	C	THR	B	189	14.672	37.080	58.963	1.00	9.79
8827	O	THR	B	189	13.688	36.353	58.872	1.00	9.52
8828	N	GLY	B	190	14.597	38.408	58.994	1.00	9.95
8830	CA	GLY	B	190	13.344	39.117	58.810	1.00	10.15
8833	C	GLY	B	190	12.628	39.500	60.095	1.00	10.36
8834	O	GLY	B	190	11.618	40.190	60.043	1.00	10.54
8835	N	HIS	B	191	13.138	39.050	61.241	1.00	10.44
8837	CA	HIS	B	191	12.617	39.458	62.543	1.00	10.52
8839	CB	HIS	B	191	12.689	38.304	63.547	1.00	10.55
8842	CG	HIS	B	191	11.533	37.359	63.462	1.00	11.04
8843	ND1	HIS	B	191	10.761	37.030	64.555	1.00	12.34
8845	CE1	HIS	B	191	9.814	36.187	64.183	1.00	12.73
8847	NE2	HIS	B	191	9.947	35.954	62.890	1.00	12.17
8849	CD2	HIS	B	191	11.014	36.677	62.415	1.00	11.49
8851	C	HIS	B	191	13.460	40.624	63.057	1.00	10.51
8852	O	HIS	B	191	14.652	40.446	63.270	1.00	9.95
8853	N	PRO	B	192	12.868	41.806	63.249	1.00	10.76
8854	CA	PRO	B	192	13.615	42.939	63.817	1.00	10.88
8856	CB	PRO	B	192	12.620	44.108	63.730	1.00	11.03
8859	CG	PRO	B	192	11.286	43.484	63.617	1.00	11.25
8862	CD	PRO	B	192	11.477	42.170	62.925	1.00	11.00
8865	C	PRO	B	192	14.068	42.718	65.265	1.00	10.79
8866	O	PRO	B	192	15.092	43.280	65.651	1.00	10.64
8867	N	TYR	B	193	13.327	41.917	66.033	1.00	10.86
8869	CA	TYR	B	193	13.650	41.634	67.439	1.00	11.09
8871	CB	TYR	B	193	12.509	42.086	68.356	1.00	11.46
8874	CG	TYR	B	193	11.981	43.469	68.061	1.00	13.13
8875	CD1	TYR	B	193	10.676	43.659	67.611	1.00	14.74
8877	CE1	TYR	B	193	10.186	44.937	67.339	1.00	16.26
8879	CZ	TYR	B	193	11.008	46.037	67.517	1.00	16.72
8880	OH	TYR	B	193	10.534	47.300	67.252	1.00	17.61
8882	CE2	TYR	B	193	12.306	45.873	67.965	1.00	16.67
8884	CD2	TYR	B	193	12.786	44.588	68.233	1.00	15.72
8886	C	TYR	B	193	13.892	40.140	67.658	1.00	10.71
8887	O	TYR	B	193	13.401	39.313	66.886	1.00	10.63
8888	N	PRO	B	194	14.633	39.784	68.706	1.00	10.34
8889	CA	PRO	B	194	14.917	38.373	68.978	1.00	10.19
8891	CB	PRO	B	194	15.898	38.426	70.158	1.00	10.18
8894	CG	PRO	B	194	16.396	39.824	70.207	1.00	10.24
8897	CD	PRO	B	194	15.277	40.664	69.699	1.00	10.35
8900	C	PRO	B	194	13.684	37.549	69.365	1.00	10.14
8901	O	PRO	B	194	12.703	38.076	69.895	1.00	9.72
8902	N	MSE	B	195	13.750	36.261	69.050	1.00	10.14
8904	CA	MSE	B	195	12.901	35.249	69.653	1.00	10.49
8906	CB	MSE	B	195	12.738	34.058	68.707	1.00	10.74
8909	CG	MSE	B	195	12.073	34.392	67.384	1.00	11.07
8912	SE	MSE	B	195	10.177	34.760	67.603	1.00	13.09
8913	CE	MSE	B	195	9.544	32.978	67.987	1.00	12.65
8917	C	MSE	B	195	13.628	34.798	70.909	1.00	10.58
8918	O	MSE	B	195	14.829	34.538	70.868	1.00	10.57
8919	N	VAL	B	196	12.913	34.701	72.021	1.00	10.39

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8921	CA	VAL	B	196	13.537	34.328	73.282	1.00	10.26
8923	CB	VAL	B	196	14.055	35.582	74.049	1.00	10.35
8925	CG1	VAL	B	196	12.913	36.531	74.417	1.00	10.25
8929	CG2	VAL	B	196	14.856	35.177	75.287	1.00	10.28
8933	C	VAL	B	196	12.608	33.475	74.150	1.00	10.31
8934	O	VAL	B	196	11.414	33.747	74.289	1.00	10.04
8935	N	ASP	B	197	13.176	32.397	74.671	1.00	10.15
8937	CA	ASP	B	197	12.594	31.640	75.759	1.00	10.09
8939	CB	ASP	B	197	12.816	30.152	75.505	1.00	10.19
8942	CG	ASP	B	197	12.154	29.271	76.542	1.00	10.28
8943	OD1	ASP	B	197	12.057	29.679	77.717	1.00	10.15
8944	OD2	ASP	B	197	11.710	28.143	76.263	1.00	10.51
8945	C	ASP	B	197	13.315	32.109	77.020	1.00	10.20
8946	O	ASP	B	197	14.418	31.649	77.314	1.00	9.95
8947	N	GLY	B	198	12.693	33.032	77.752	1.00	9.99
8949	CA	GLY	B	198	13.282	33.627	78.942	1.00	10.14
8952	C	GLY	B	198	13.901	32.648	79.933	1.00	10.20
8953	O	GLY	B	198	15.113	32.688	80.149	1.00	9.77
8954	N	PRO	B	199	13.086	31.791	80.552	1.00	10.11
8955	CA	PRO	B	199	13.603	30.768	81.473	1.00	10.10
8957	CB	PRO	B	199	12.358	29.937	81.818	1.00	10.28
8960	CG	PRO	B	199	11.213	30.908	81.662	1.00	10.47
8963	CD	PRO	B	199	11.612	31.772	80.475	1.00	10.38
8966	C	PRO	B	199	14.715	29.886	80.891	1.00	10.07
8967	O	PRO	B	199	15.674	29.596	81.603	1.00	9.92
8968	N	LEU	B	200	14.600	29.476	79.630	1.00	9.92
8970	CA	LEU	B	200	15.614	28.620	79.016	1.00	9.83
8972	CB	LEU	B	200	15.137	28.075	77.668	1.00	9.79
8975	CG	LEU	B	200	16.108	27.145	76.928	1.00	9.73
8977	CD1	LEU	B	200	15.502	26.702	75.621	1.00	9.92
8981	CD2	LEU	B	200	16.486	25.932	77.781	1.00	10.51
8985	C	LEU	B	200	16.941	29.354	78.831	1.00	9.83
8986	O	LEU	B	200	18.003	28.759	78.982	1.00	9.84
8987	N	SER	B	201	16.878	30.639	78.493	1.00	9.86
8989	CA	SER	B	201	18.083	31.440	78.313	1.00	10.06
8991	CB	SER	B	201	17.742	32.808	77.702	1.00	9.89
8994	OG	SER	B	201	17.047	33.645	78.613	1.00	9.75
8996	C	SER	B	201	18.827	31.577	79.638	1.00	10.33
8997	O	SER	B	201	20.050	31.449	79.682	1.00	10.35
8998	N	ASN	B	202	18.084	31.812	80.717	1.00	10.88
9000	CA	ASN	B	202	18.664	31.897	82.058	1.00	11.24
9002	CB	ASN	B	202	17.584	32.229	83.097	1.00	11.29
9005	CG	ASN	B	202	17.182	33.697	83.088	1.00	11.75
9006	OD1	ASN	B	202	17.863	34.550	82.507	1.00	12.97
9007	ND2	ASN	B	202	16.067	33.999	83.743	1.00	11.90
9010	C	ASN	B	202	19.357	30.596	82.451	1.00	11.46
9011	O	ASN	B	202	20.502	30.596	82.901	1.00	11.23
9012	N	GLU	B	203	18.650	29.490	82.267	1.00	11.84
9014	CA	GLU	B	203	19.162	28.181	82.636	1.00	12.22
9016	CB	GLU	B	203	18.064	27.132	82.516	1.00	12.86
9019	CG	GLU	B	203	18.513	25.722	82.854	1.00	15.31
9022	CD	GLU	B	203	17.407	24.718	82.650	1.00	18.80

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9023	OE1	GLU	B	203	17.148	24.351	81.481	1.00	21.49
9024	OE2	GLU	B	203	16.798	24.305	83.659	1.00	22.29
9025	C	GLU	B	203	20.351	27.776	81.778	1.00	11.66
9026	O	GLU	B	203	21.295	27.191	82.291	1.00	11.26
9027	N	THR	B	204	20.304	28.084	80.482	1.00	10.99
9029	CA	THR	B	204	21.374	27.689	79.564	1.00	10.84
9031	CB	THR	B	204	20.956	27.898	78.089	1.00	10.85
9033	OG1	THR	B	204	19.755	27.165	77.812	1.00	10.56
9035	CG2	THR	B	204	21.978	27.294	77.139	1.00	10.68
9039	C	THR	B	204	22.648	28.469	79.878	1.00	10.59
9040	O	THR	B	204	23.742	27.923	79.815	1.00	10.43
9041	N	TYR	B	205	22.490	29.742	80.229	1.00	10.47
9043	CA	TYR	B	205	23.596	30.573	80.706	1.00	10.60
9045	CB	TYR	B	205	23.079	31.983	81.033	1.00	10.44
9048	CG	TYR	B	205	24.126	32.991	81.492	1.00	10.65
9049	CD1	TYR	B	205	24.762	32.861	82.725	1.00	9.88
9051	CE1	TYR	B	205	25.700	33.787	83.154	1.00	10.12
9053	CZ	TYR	B	205	26.004	34.870	82.360	1.00	10.48
9054	OH	TYR	B	205	26.933	35.793	82.786	1.00	9.44
9056	CE2	TYR	B	205	25.379	35.037	81.141	1.00	10.98
9058	CD2	TYR	B	205	24.442	34.102	80.712	1.00	10.82
9060	C	TYR	B	205	24.247	29.942	81.943	1.00	10.76
9061	O	TYR	B	205	25.458	29.751	81.981	1.00	10.45
9062	N	ILE	B	206	23.431	29.635	82.950	1.00	11.19
9064	CA	ILE	B	206	23.925	29.092	84.219	1.00	11.73
9066	CB	ILE	B	206	22.773	28.940	85.246	1.00	11.97
9068	CG1	ILE	B	206	22.347	30.320	85.743	1.00	12.38
9071	CD1	ILE	B	206	21.041	30.331	86.502	1.00	13.48
9075	CG2	ILE	B	206	23.200	28.078	86.447	1.00	12.40
9079	C	ILE	B	206	24.638	27.765	84.008	1.00	11.82
9080	O	ILE	B	206	25.745	27.569	84.507	1.00	11.94
9081	N	GLN	B	207	24.007	26.868	83.256	1.00	11.84
9083	CA	GLN	B	207	24.556	25.537	83.025	1.00	12.03
9085	CB	GLN	B	207	23.484	24.607	82.456	1.00	12.52
9088	CG	GLN	B	207	22.394	24.285	83.478	1.00	14.35
9091	CD	GLN	B	207	21.295	23.395	82.932	1.00	17.08
9092	OE1	GLN	B	207	21.329	22.994	81.766	1.00	19.51
9093	NE2	GLN	B	207	20.318	23.073	83.780	1.00	17.97
9096	C	GLN	B	207	25.783	25.576	82.122	1.00	11.30
9097	O	GLN	B	207	26.663	24.735	82.245	1.00	10.77
9098	N	SER	B	208	25.848	26.562	81.231	1.00	10.63
9100	CA	SER	B	208	26.998	26.708	80.350	1.00	10.21
9102	CB	ASER	B	208	26.710	27.681	79.204	0.65	9.93
9105	OG	ASER	B	208	25.793	27.110	78.294	0.65	9.20
9107	C	SER	B	208	28.206	27.165	81.155	1.00	10.16
9108	O	SER	B	208	29.296	26.638	80.978	1.00	9.71
9109	N	PHE	B	209	28.007	28.134	82.046	1.00	10.49
9111	CA	PHE	B	209	29.072	28.565	82.946	1.00	10.78
9113	CB	PHE	B	209	28.636	29.724	83.843	1.00	10.84
9116	CG	PHE	B	209	29.625	30.031	84.928	1.00	11.05
9117	CD1	PHE	B	209	29.313	29.811	86.262	1.00	11.55
9119	CE1	PHE	B	209	30.247	30.071	87.260	1.00	11.85

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9121	CZ	PHE	B	209	31.507	30.545	86.926	1.00	11.34
9123	CE2	PHE	B	209	31.831	30.756	85.598	1.00	11.62
9125	CD2	PHE	B	209	30.892	30.495	84.606	1.00	11.03
9127	C	PHE	B	209	29.541	27.403	83.815	1.00	11.02
9128	O	PHE	B	209	30.733	27.159	83.934	1.00	10.70
9129	N	ALA	B	210	28.592	26.686	84.411	1.00	11.43
9131	CA	ALA	B	210	28.900	25.519	85.236	1.00	11.46
9133	CB	ALA	B	210	27.609	24.859	85.733	1.00	11.48
9137	C	ALA	B	210	29.751	24.500	84.480	1.00	11.49
9138	O	ALA	B	210	30.680	23.928	85.038	1.00	11.30
9139	N	GLN	B	211	29.430	24.287	83.207	1.00	11.73
9141	CA	GLN	B	211	30.103	23.273	82.392	1.00	11.75
9143	CB	GLN	B	211	29.298	22.982	81.117	1.00	12.08
9146	CG	GLN	B	211	28.138	22.018	81.324	1.00	13.53
9149	CD	GLN	B	211	27.330	21.794	80.053	1.00	15.53
9150	OE1	GLN	B	211	27.745	21.030	79.182	1.00	16.93
9151	NE2	GLN	B	211	26.179	22.454	79.949	1.00	17.13
9154	C	GLN	B	211	31.538	23.681	82.033	1.00	11.37
9155	O	GLN	B	211	32.463	22.885	82.196	1.00	10.85
9156	N	VAL	B	212	31.718	24.905	81.535	1.00	11.01
9158	CA	VAL	B	212	33.060	25.403	81.202	1.00	11.02
9160	CB	VAL	B	212	33.056	26.684	80.305	1.00	11.00
9162	CG1	VAL	B	212	32.430	26.391	78.944	1.00	11.04
9166	CG2	VAL	B	212	32.363	27.860	80.996	1.00	11.14
9170	C	VAL	B	212	33.913	25.656	82.444	1.00	10.89
9171	O	VAL	B	212	35.118	25.433	82.407	1.00	10.90
9172	N	TRP	B	213	33.300	26.117	83.533	1.00	10.70
9174	CA	TRP	B	213	34.015	26.274	84.798	1.00	10.74
9176	CB	TRP	B	213	33.140	26.914	85.887	1.00	10.73
9179	CG	TRP	B	213	33.807	26.876	87.231	1.00	10.43
9180	CD1	TRP	B	213	33.551	26.002	88.256	1.00	10.48
9182	NE1	TRP	B	213	34.388	26.257	89.316	1.00	9.70
9184	CE2	TRP	B	213	35.207	27.309	88.996	1.00	10.64
9185	CD2	TRP	B	213	34.871	27.721	87.686	1.00	10.61
9186	CE3	TRP	B	213	35.578	28.792	87.122	1.00	10.97
9188	CZ3	TRP	B	213	36.575	29.407	87.867	1.00	10.75
9190	CH2	TRP	B	213	36.880	28.976	89.166	1.00	10.94
9192	CZ2	TRP	B	213	36.209	27.932	89.747	1.00	10.64
9194	C	TRP	B	213	34.530	24.923	85.295	1.00	10.84
9195	O	TRP	B	213	35.706	24.788	85.610	1.00	10.48
9196	N	ASP	B	214	33.638	23.938	85.366	1.00	11.22
9198	CA	ASP	B	214	33.980	22.604	85.873	1.00	11.47
9200	CB	ASP	B	214	32.761	21.677	85.874	1.00	11.54
9203	CG	ASP	B	214	31.807	21.953	87.019	1.00	12.06
9204	OD1	ASP	B	214	30.670	21.438	86.970	1.00	12.44
9205	OD2	ASP	B	214	32.093	22.667	87.998	1.00	13.30
9206	C	ASP	B	214	35.081	21.955	85.044	1.00	11.41
9207	O	ASP	B	214	35.990	21.357	85.595	1.00	11.27
9208	N	GLU	B	215	34.982	22.074	83.722	1.00	11.45
9210	CA	GLU	B	215	35.971	21.509	82.814	1.00	11.61
9212	CB	GLU	B	215	35.457	21.545	81.370	1.00	11.65
9215	CG	GLU	B	215	36.429	21.019	80.319	1.00	11.36

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9218	CD	GLU	B	215	36.727	19.531	80.456	1.00	11.18
9219	OE1	GLU	B	215	37.751	19.077	79.910	1.00	11.70
9220	OE2	GLU	B	215	35.949	18.811	81.097	1.00	10.36
9221	C	GLU	B	215	37.297	22.258	82.924	1.00	11.95
9222	O	GLU	B	215	38.360	21.648	82.832	1.00	12.01
9223	N	HIS	B	216	37.227	23.573	83.119	1.00	12.30
9225	CA	HIS	B	216	38.416	24.402	83.310	1.00	12.71
9227	CB	HIS	B	216	38.047	25.895	83.357	1.00	12.59
9230	CG	HIS	B	216	39.231	26.807	83.477	1.00	12.79
9231	ND1	HIS	B	216	39.852	27.066	84.678	1.00	12.83
9233	CE1	HIS	B	216	40.865	27.891	84.480	1.00	13.09
9235	NE2	HIS	B	216	40.919	28.183	83.193	1.00	12.89
9237	CD2	HIS	B	216	39.907	27.519	82.543	1.00	13.40
9239	C	HIS	B	216	39.149	24.003	84.589	1.00	12.95
9240	O	HIS	B	216	40.370	23.879	84.589	1.00	12.95
9241	N	LYS	B	217	38.395	23.805	85.668	1.00	13.35
9243	CA	LYS	B	217	38.960	23.412	86.962	1.00	13.93
9245	CB	LYS	B	217	37.885	23.487	88.061	1.00	14.05
9248	CG	LYS	B	217	38.318	22.954	89.427	1.00	14.68
9251	CD	LYS	B	217	37.337	23.336	90.540	1.00	16.39
9254	CE	LYS	B	217	36.056	22.518	90.495	1.00	17.54
9257	NZ	LYS	B	217	35.481	22.303	91.856	1.00	19.01
9261	C	LYS	B	217	39.540	22.000	86.866	1.00	14.16
9262	O	LYS	B	217	40.619	21.724	87.378	1.00	14.11
9263	N	LYS	B	218	38.814	21.121	86.187	1.00	14.66
9265	CA	LYS	B	218	39.253	19.752	85.929	1.00	15.16
9267	CB	LYS	B	218	38.184	19.041	85.091	1.00	15.50
9270	CG	LYS	B	218	38.453	17.593	84.732	1.00	16.41
9273	CD	LYS	B	218	37.209	16.998	84.084	1.00	18.09
9276	CE	LYS	B	218	37.437	15.568	83.648	1.00	19.19
9279	NZ	LYS	B	218	38.339	15.500	82.479	1.00	20.49
9283	C	LYS	B	218	40.616	19.705	85.229	1.00	15.21
9284	O	LYS	B	218	41.469	18.887	85.582	1.00	15.77
9285	N	ARG	B	219	40.828	20.606	84.269	1.00	15.02
9287	CA	ARG	B	219	42.048	20.627	83.455	1.00	14.88
9289	CB	ARG	B	219	41.786	21.341	82.120	1.00	15.16
9292	CG	ARG	B	219	40.966	20.572	81.082	1.00	15.82
9295	CD	ARG	B	219	40.768	21.374	79.787	1.00	16.72
9298	NE	ARG	B	219	39.757	20.810	78.892	1.00	17.91
9300	CZ	ARG	B	219	39.388	21.361	77.728	1.00	18.69
9301	NH1	ARG	B	219	38.454	20.776	76.987	1.00	19.32
9304	NH2	ARG	B	219	39.956	22.481	77.289	1.00	18.71
9307	C	ARG	B	219	43.248	21.319	84.124	1.00	14.55
9308	O	ARG	B	219	44.387	20.889	83.946	1.00	14.82
9309	N	THR	B	220	42.987	22.394	84.868	1.00	13.83
9311	CA	THR	B	220	44.032	23.312	85.348	1.00	13.14
9313	CB	THR	B	220	43.661	24.773	84.998	1.00	13.19
9315	OG1	THR	B	220	42.459	25.158	85.684	1.00	12.44
9317	CG2	THR	B	220	43.329	24.940	83.509	1.00	13.21
9321	C	THR	B	220	44.296	23.251	86.856	1.00	12.67
9322	O	THR	B	220	45.337	23.696	87.316	1.00	12.48
9323	N	GLY	B	221	43.339	22.734	87.620	1.00	12.42

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9325	CA	GLY	B	221	43.407	22.752	89.071	1.00	12.41
9328	C	GLY	B	221	43.177	24.117	89.707	1.00	12.24
9329	O	GLY	B	221	43.396	24.277	90.906	1.00	11.95
9330	N	LEU	B	222	42.727	25.091	88.917	1.00	12.05
9332	CA	LEU	B	222	42.446	26.435	89.419	1.00	12.30
9334	CB	LEU	B	222	42.670	27.481	88.324	1.00	12.36
9337	CG	LEU	B	222	44.091	27.519	87.756	1.00	13.59
9339	CD1	LEU	B	222	44.129	28.289	86.436	1.00	14.04
9343	CD2	LEU	B	222	45.071	28.113	88.771	1.00	14.36
9347	C	LEU	B	222	41.012	26.498	89.911	1.00	12.13
9348	O	LEU	B	222	40.094	26.087	89.200	1.00	11.85
9349	N	ASP	B	223	40.833	26.994	91.135	1.00	12.02
9351	CA	ASP	B	223	39.519	27.138	91.754	1.00	12.14
9353	CB	ASP	B	223	39.471	26.342	93.068	1.00	11.93
9356	CG	ASP	B	223	38.082	25.790	93.384	1.00	11.97
9357	OD1	ASP	B	223	37.987	24.833	94.183	1.00	11.89
9358	OD2	ASP	B	223	37.031	26.247	92.899	1.00	10.32
9359	C	ASP	B	223	39.239	28.631	91.984	1.00	12.32
9360	O	ASP	B	223	40.058	29.477	91.634	1.00	12.25
9361	N	PHE	B	224	38.086	28.948	92.569	1.00	12.69
9363	CA	PHE	B	224	37.647	30.336	92.745	1.00	13.02
9365	CB	PHE	B	224	36.286	30.373	93.443	1.00	13.24
9368	CG	PHE	B	224	35.153	29.902	92.577	1.00	13.94
9369	CD1	PHE	B	224	34.698	30.690	91.531	1.00	14.51
9371	CE1	PHE	B	224	33.655	30.263	90.720	1.00	15.63
9373	CZ	PHE	B	224	33.058	29.032	90.951	1.00	15.40
9375	CE2	PHE	B	224	33.507	28.234	91.993	1.00	15.09
9377	CD2	PHE	B	224	34.551	28.670	92.800	1.00	14.33
9379	C	PHE	B	224	38.646	31.202	93.512	1.00	13.10
9380	O	PHE	B	224	38.813	32.376	93.201	1.00	13.05
9381	N	ALA	B	225	39.319	30.610	94.494	1.00	13.22
9383	CA	ALA	B	225	40.250	31.336	95.360	1.00	13.27
9385	CB	ALA	B	225	40.488	30.553	96.640	1.00	13.53
9389	C	ALA	B	225	41.584	31.649	94.678	1.00	13.23
9390	O	ALA	B	225	42.364	32.459	95.184	1.00	13.13
9391	N	ASP	B	226	41.849	30.999	93.546	1.00	12.84
9393	CA	ASP	B	226	42.994	31.335	92.701	1.00	12.64
9395	CB	ASP	B	226	43.405	30.119	91.872	1.00	12.88
9398	CG	ASP	B	226	43.757	28.935	92.738	1.00	13.26
9399	OD1	ASP	B	226	43.252	27.830	92.485	1.00	13.56
9400	OD2	ASP	B	226	44.516	29.029	93.715	1.00	13.82
9401	C	ASP	B	226	42.721	32.520	91.772	1.00	12.31
9402	O	ASP	B	226	43.640	33.031	91.136	1.00	12.04
9403	N	TYR	B	227	41.459	32.937	91.688	1.00	11.92
9405	CA	TYR	B	227	41.071	34.098	90.898	1.00	11.80
9407	CB	TYR	B	227	39.820	33.787	90.073	1.00	11.60
9410	CG	TYR	B	227	40.164	32.964	88.860	1.00	11.30
9411	CD1	TYR	B	227	40.058	31.571	88.879	1.00	10.87
9413	CE1	TYR	B	227	40.400	30.815	87.763	1.00	10.94
9415	CZ	TYR	B	227	40.872	31.460	86.628	1.00	10.42
9416	OH	TYR	B	227	41.227	30.747	85.511	1.00	10.39
9418	CE2	TYR	B	227	40.998	32.834	86.602	1.00	10.76

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9420	CD2	TYR	B	227	40.647	33.575	87.709	1.00	10.43
9422	C	TYR	B	227	40.840	35.309	91.788	1.00	11.87
9423	O	TYR	B	227	40.184	35.219	92.820	1.00	11.61
9424	N	ASP	B	228	41.407	36.437	91.381	1.00	12.06
9426	CA	ASP	B	228	41.164	37.703	92.055	1.00	12.40
9428	CB	ASP	B	228	42.321	38.657	91.787	1.00	12.45
9431	CG	ASP	B	228	43.646	38.081	92.245	1.00	13.07
9432	OD1	ASP	B	228	43.906	38.090	93.465	1.00	13.16
9433	OD2	ASP	B	228	44.472	37.569	91.465	1.00	12.77
9434	C	ASP	B	228	39.831	38.301	91.617	1.00	12.35
9435	O	ASP	B	228	39.200	39.038	92.366	1.00	12.19
9436	N	ALA	B	229	39.398	37.976	90.402	1.00	12.37
9438	CA	ALA	B	229	38.078	38.388	89.935	1.00	12.31
9440	CB	ALA	B	229	38.113	39.839	89.468	1.00	12.24
9444	C	ALA	B	229	37.570	37.491	88.818	1.00	12.51
9445	O	ALA	B	229	38.354	36.891	88.088	1.00	12.16
9446	N	LEU	B	230	36.247	37.402	88.711	1.00	12.87
9448	CA	LEU	B	230	35.575	36.737	87.597	1.00	13.18
9450	CB	LEU	B	230	34.811	35.496	88.070	1.00	13.40
9453	CG	LEU	B	230	35.655	34.314	88.566	1.00	14.93
9455	CD1	LEU	B	230	34.751	33.150	88.953	1.00	16.11
9459	CD2	LEU	B	230	36.668	33.873	87.525	1.00	15.46
9463	C	LEU	B	230	34.606	37.728	86.965	1.00	12.98
9464	O	LEU	B	230	33.681	38.209	87.628	1.00	13.35
9465	N	ALA	B	231	34.845	38.052	85.697	1.00	12.47
9467	CA	ALA	B	231	33.966	38.908	84.912	1.00	11.96
9469	CB	ALA	B	231	34.775	39.866	84.082	1.00	12.13
9473	C	ALA	B	231	33.099	38.037	84.013	1.00	11.63
9474	O	ALA	B	231	33.562	37.032	83.472	1.00	11.43
9475	N	PHE	B	232	31.847	38.444	83.856	1.00	10.96
9477	CA	PHE	B	232	30.842	37.671	83.145	1.00	10.45
9479	CB	PHE	B	232	29.731	37.250	84.109	1.00	10.39
9482	CG	PHE	B	232	30.135	36.181	85.087	1.00	10.02
9483	CD1	PHE	B	232	29.734	34.864	84.897	1.00	10.15
9485	CE1	PHE	B	232	30.090	33.873	85.801	1.00	10.15
9487	CZ	PHE	B	232	30.842	34.192	86.911	1.00	9.24
9489	CE2	PHE	B	232	31.244	35.501	87.121	1.00	10.42
9491	CD2	PHE	B	232	30.879	36.497	86.210	1.00	9.64
9493	C	PHE	B	232	30.207	38.510	82.057	1.00	10.11
9494	O	PHE	B	232	30.177	39.740	82.137	1.00	9.51
9495	N	HIS	B	233	29.676	37.826	81.052	1.00	9.65
9497	CA	HIS	B	233	28.726	38.423	80.133	1.00	9.55
9499	CB	HIS	B	233	28.221	37.365	79.159	1.00	9.43
9502	CG	HIS	B	233	27.075	37.816	78.317	1.00	9.44
9503	ND1	HIS	B	233	27.225	38.709	77.281	1.00	9.43
9505	CE1	HIS	B	233	26.050	38.923	76.718	1.00	10.27
9507	NE2	HIS	B	233	25.142	38.207	77.356	1.00	9.92
9509	CD2	HIS	B	233	25.757	37.508	78.363	1.00	9.87
9511	C	HIS	B	233	27.564	38.966	80.961	1.00	9.54
9512	O	HIS	B	233	27.012	38.251	81.796	1.00	9.46
9513	N	ILE	B	234	27.226	40.237	80.752	1.00	9.46
9515	CA	ILE	B	234	26.168	40.901	81.517	1.00	9.58

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9517	CB	ILE	B	234	26.711	42.167	82.238	1.00	9.69
9519	CG1	ILE	B	234	27.935	41.832	83.093	1.00	10.53
9522	CD1	ILE	B	234	28.853	43.025	83.350	1.00	11.26
9526	CG2	ILE	B	234	25.629	42.780	83.134	1.00	9.85
9530	C	ILE	B	234	24.970	41.270	80.626	1.00	9.38
9531	O	ILE	B	234	24.897	42.384	80.103	1.00	9.22
9532	N	PRO	B	235	24.023	40.347	80.467	1.00	9.19
9533	CA	PRO	B	235	22.780	40.647	79.746	1.00	9.31
9535	CB	PRO	B	235	22.176	39.265	79.498	1.00	9.11
9538	CG	PRO	B	235	22.689	38.414	80.622	1.00	9.23
9541	CD	PRO	B	235	24.036	38.967	80.989	1.00	9.32
9544	C	PRO	B	235	21.870	41.477	80.637	1.00	9.27
9545	O	PRO	B	235	21.117	42.339	80.195	1.00	9.40
9546	N	TYR	B	236	21.927	41.135	81.912	1.00	9.51
9548	CA	TYR	B	236	21.474	41.979	82.986	1.00	9.69
9550	CB	TYR	B	236	19.975	41.835	83.239	1.00	9.64
9553	CG	TYR	B	236	19.480	40.433	83.509	1.00	9.86
9554	CD1	TYR	B	236	19.296	39.979	84.812	1.00	9.65
9556	CE1	TYR	B	236	18.822	38.703	85.068	1.00	10.77
9558	CZ	TYR	B	236	18.510	37.864	84.015	1.00	10.56
9559	OH	TYR	B	236	18.035	36.599	84.276	1.00	12.52
9561	CE2	TYR	B	236	18.673	38.294	82.711	1.00	10.29
9563	CD2	TYR	B	236	19.149	39.578	82.465	1.00	10.48
9565	C	TYR	B	236	22.296	41.606	84.206	1.00	9.87
9566	O	TYR	B	236	22.907	40.543	84.290	1.00	9.76
9567	N	THR	B	237	22.286	42.505	85.161	1.00	10.01
9569	CA	THR	B	237	23.284	42.547	86.200	1.00	10.41
9571	CB	THR	B	237	23.126	43.941	86.863	1.00	10.73
9573	OG1	THR	B	237	24.192	44.811	86.445	1.00	12.28
9575	CG2	THR	B	237	23.168	43.901	88.323	1.00	10.41
9579	C	THR	B	237	23.183	41.345	87.169	1.00	10.48
9580	O	THR	B	237	24.196	40.837	87.656	1.00	10.20
9581	N	LYS	B	238	21.969	40.859	87.402	1.00	10.60
9583	CA	LYS	B	238	21.768	39.712	88.284	1.00	11.06
9585	CB	LYS	B	238	20.328	39.688	88.815	1.00	11.36
9588	CG	LYS	B	238	20.075	40.664	89.953	1.00	12.65
9591	CD	LYS	B	238	20.697	40.181	91.264	1.00	14.34
9594	CE	LYS	B	238	20.327	41.074	92.454	1.00	15.41
9597	NZ	LYS	B	238	20.268	42.537	92.119	1.00	16.16
9601	C	LYS	B	238	22.103	38.367	87.631	1.00	11.04
9602	O	LYS	B	238	22.213	37.364	88.329	1.00	10.95
9603	N	MSE	B	239	22.260	38.334	86.308	1.00	11.06
9605	CA	MSE	B	239	22.489	37.072	85.599	1.00	11.30
9607	CB	MSE	B	239	22.501	37.288	84.080	1.00	11.48
9610	CG	MSE	B	239	22.619	35.995	83.280	1.00	11.86
9613	SE	MSE	B	239	21.003	34.920	83.420	1.00	13.22
9614	CE	MSE	B	239	21.628	33.500	84.587	1.00	13.65
9618	C	MSE	B	239	23.789	36.400	86.026	1.00	11.42
9619	O	MSE	B	239	23.797	35.227	86.406	1.00	11.28
9620	N	GLY	B	240	24.884	37.148	85.957	1.00	11.70
9622	CA	GLY	B	240	26.185	36.640	86.342	1.00	11.90
9625	C	GLY	B	240	26.202	36.261	87.809	1.00	12.32

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9626	O	GLY	B	240	26.809	35.258	88.182	1.00	12.10
9627	N	LYS	B	241	25.526	37.054	88.638	1.00	12.67
9629	CA	LYS	B	241	25.439	36.755	90.064	1.00	13.33
9631	CB	LYS	B	241	24.703	37.855	90.838	1.00	13.49
9634	CG	LYS	B	241	24.996	37.802	92.328	1.00	14.46
9637	CD	LYS	B	241	24.093	38.700	93.136	1.00	15.93
9640	CE	LYS	B	241	24.395	38.583	94.621	1.00	16.69
9643	NZ	LYS	B	241	23.324	39.191	95.457	1.00	17.43
9647	C	LYS	B	241	24.762	35.412	90.317	1.00	13.31
9648	O	LYS	B	241	25.223	34.648	91.153	1.00	13.59
9649	N	LYS	B	242	23.685	35.125	89.595	1.00	13.43
9651	CA	LYS	B	242	22.974	33.851	89.734	1.00	13.58
9653	CB	LYS	B	242	21.699	33.844	88.885	1.00	13.58
9656	CG	LYS	B	242	20.546	34.641	89.490	1.00	13.46
9659	CD	LYS	B	242	19.260	34.464	88.697	1.00	13.68
9662	CE	LYS	B	242	19.318	35.149	87.339	1.00	13.49
9665	NZ	LYS	B	242	18.020	35.052	86.623	1.00	12.97
9669	C	LYS	B	242	23.852	32.660	89.348	1.00	13.76
9670	O	LYS	B	242	23.845	31.634	90.029	1.00	13.68
9671	N	ALA	B	243	24.599	32.797	88.255	1.00	13.88
9673	CA	ALA	B	243	25.510	31.749	87.795	1.00	14.31
9675	CB	ALA	B	243	26.128	32.139	86.454	1.00	14.25
9679	C	ALA	B	243	26.608	31.505	88.829	1.00	14.55
9680	O	ALA	B	243	26.975	30.362	89.113	1.00	14.25
9681	N	LEU	B	244	27.104	32.600	89.395	1.00	15.17
9683	CA	LEU	B	244	28.164	32.575	90.396	1.00	15.68
9685	CB	LEU	B	244	28.638	34.010	90.678	1.00	15.95
9688	CG	LEU	B	244	30.040	34.265	91.227	1.00	16.54
9690	CD1	LEU	B	244	31.084	33.413	90.532	1.00	16.65
9694	CD2	LEU	B	244	30.368	35.751	91.089	1.00	17.30
9698	C	LEU	B	244	27.669	31.907	91.679	1.00	15.97
9699	O	LEU	B	244	28.309	30.994	92.189	1.00	16.02
9700	N	LEU	B	245	26.514	32.353	92.173	1.00	16.37
9702	CA	LEU	B	245	25.910	31.817	93.396	1.00	16.67
9704	CB	LEU	B	245	24.583	32.527	93.701	1.00	16.81
9707	CG	LEU	B	245	24.663	33.950	94.269	1.00	17.19
9709	CD1	LEU	B	245	23.293	34.612	94.197	1.00	17.78
9713	CD2	LEU	B	245	25.187	33.960	95.702	1.00	16.92
9717	C	LEU	B	245	25.667	30.309	93.322	1.00	16.87
9718	O	LEU	B	245	25.772	29.611	94.329	1.00	16.98
9719	N	ALA	B	246	25.356	29.811	92.128	1.00	16.87
9721	CA	ALA	B	246	25.081	28.390	91.933	1.00	16.98
9723	CB	ALA	B	246	24.443	28.163	90.568	1.00	17.00
9727	C	ALA	B	246	26.326	27.507	92.087	1.00	17.08
9728	O	ALA	B	246	26.197	26.299	92.285	1.00	17.26
9729	N	LYS	B	247	27.517	28.104	91.993	1.00	17.02
9731	CA	LYS	B	247	28.778	27.357	92.017	1.00	17.11
9733	CB	LYS	B	247	29.562	27.634	90.725	1.00	17.29
9736	CG	LYS	B	247	28.890	27.154	89.446	1.00	17.21
9739	CD	LYS	B	247	28.682	25.640	89.405	1.00	17.61
9742	CE	LYS	B	247	29.958	24.884	89.068	1.00	18.09
9745	NZ	LYS	B	247	29.822	23.424	89.351	1.00	17.65

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9749	C	LYS	B	247	29.707	27.616	93.213	1.00	17.17
9750	O	LYS	B	247	30.620	26.830	93.442	1.00	17.01
9751	N	ILE	B	248	29.490	28.695	93.967	1.00	17.30
9753	CA	ILE	B	248	30.420	29.083	95.040	1.00	17.63
9755	CB	ILE	B	248	30.757	30.604	94.963	1.00	17.44
9757	CG1	ILE	B	248	29.527	31.464	95.300	1.00	17.33
9760	CD1	ILE	B	248	29.787	32.965	95.291	1.00	17.80
9764	CG2	ILE	B	248	31.338	30.946	93.598	1.00	17.61
9768	C	ILE	B	248	29.942	28.736	96.456	1.00	18.10
9769	O	ILE	B	248	30.551	29.172	97.432	1.00	17.86
9770	N	SER	B	249	28.867	27.960	96.569	1.00	18.95
9772	CA	SER	B	249	28.274	27.649	97.874	1.00	19.77
9774	CB	SER	B	249	26.889	27.016	97.703	1.00	19.89
9777	OG	SER	B	249	26.989	25.664	97.292	1.00	20.20
9779	C	SER	B	249	29.152	26.747	98.751	1.00	20.41
9780	O	SER	B	249	28.993	26.741	99.971	1.00	20.61
9781	N	ASP	B	250	30.062	25.987	98.136	1.00	21.13
9783	CA	ASP	B	250	31.032	25.172	98.889	1.00	21.79
9785	CB	ASP	B	250	31.341	23.834	98.177	1.00	22.12
9788	CG	ASP	B	250	31.828	23.997	96.733	1.00	23.96
9789	OD1	ASP	B	250	32.225	25.113	96.317	1.00	26.33
9790	OD2	ASP	B	250	31.849	23.030	95.934	1.00	26.36
9791	C	ASP	B	250	32.329	25.914	99.267	1.00	21.67
9792	O	ASP	B	250	33.219	25.335	99.890	1.00	21.87
9793	N	GLN	B	251	32.416	27.196	98.913	1.00	21.36
9795	CA	GLN	B	251	33.553	28.039	99.276	1.00	21.05
9797	CB	GLN	B	251	33.710	29.179	98.266	1.00	21.07
9800	CG	GLN	B	251	33.864	28.718	96.821	1.00	20.67
9803	CD	GLN	B	251	35.131	27.922	96.603	1.00	19.66
9804	OE1	GLN	B	251	36.223	28.398	96.905	1.00	19.19
9805	NE2	GLN	B	251	34.991	26.707	96.088	1.00	19.49
9808	C	GLN	B	251	33.354	28.631	100.664	1.00	21.04
9809	O	GLN	B	251	32.227	28.721	101.144	1.00	20.86
9810	N	THR	B	252	34.446	29.059	101.295	1.00	21.07
9812	CA	THR	B	252	34.368	29.679	102.618	1.00	21.21
9814	CB	THR	B	252	35.770	29.980	103.212	1.00	21.24
9816	OG1	THR	B	252	36.452	30.948	102.406	1.00	20.75
9818	CG2	THR	B	252	36.687	28.742	103.190	1.00	21.40
9822	C	THR	B	252	33.572	30.975	102.522	1.00	21.63
9823	O	THR	B	252	33.418	31.541	101.436	1.00	21.21
9824	N	GLU	B	253	33.072	31.438	103.661	1.00	21.89
9826	CA	GLU	B	253	32.294	32.666	103.705	1.00	22.40
9828	CB	GLU	B	253	31.747	32.911	105.118	1.00	22.87
9831	CG	GLU	B	253	30.769	34.079	105.227	1.00	24.62
9834	CD	GLU	B	253	29.602	33.978	104.255	1.00	26.67
9835	OE1	GLU	B	253	29.070	32.860	104.069	1.00	28.15
9836	OE2	GLU	B	253	29.220	35.020	103.673	1.00	28.42
9837	C	GLU	B	253	33.129	33.857	103.243	1.00	22.09
9838	O	GLU	B	253	32.623	34.728	102.538	1.00	22.02
9839	N	ALA	B	254	34.401	33.887	103.637	1.00	21.61
9841	CA	ALA	B	254	35.306	34.961	103.245	1.00	21.48
9843	CB	ALA	B	254	36.631	34.842	103.988	1.00	21.61

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9847	C	ALA	B	254	35.542	34.976	101.733	1.00	21.28
9848	O	ALA	B	254	35.599	36.042	101.125	1.00	21.21
9849	N	GLU	B	255	35.670	33.792	101.136	1.00	20.97
9851	CA	GLU	B	255	35.878	33.667	99.692	1.00	20.88
9853	CB	GLU	B	255	36.275	32.224	99.328	1.00	20.75
9856	CG	GLU	B	255	36.326	31.907	97.835	1.00	20.76
9859	CD	GLU	B	255	37.194	32.866	97.039	1.00	20.55
9860	OE1	GLU	B	255	38.149	33.435	97.609	1.00	19.77
9861	OE2	GLU	B	255	36.920	33.047	95.834	1.00	20.80
9862	C	GLU	B	255	34.633	34.098	98.909	1.00	20.78
9863	O	GLU	B	255	34.742	34.801	97.909	1.00	20.30
9864	N	GLN	B	256	33.461	33.669	99.370	1.00	20.90
9866	CA	GLN	B	256	32.192	34.043	98.750	1.00	21.09
9868	CB	GLN	B	256	31.015	33.369	99.466	1.00	21.04
9871	CG	GLN	B	256	30.895	31.871	99.214	1.00	20.92
9874	CD	GLN	B	256	29.707	31.247	99.935	1.00	21.13
9875	OE1	GLN	B	256	28.607	31.797	99.920	1.00	20.92
9876	NE2	GLN	B	256	29.928	30.098	100.567	1.00	21.13
9879	C	GLN	B	256	32.009	35.559	98.769	1.00	21.39
9880	O	GLN	B	256	31.587	36.143	97.777	1.00	21.13
9881	N	GLU	B	257	32.348	36.190	99.894	1.00	21.79
9883	CA	GLU	B	257	32.199	37.639	100.053	1.00	22.32
9885	CB	GLU	B	257	32.441	38.062	101.512	1.00	22.67
9888	CG	GLU	B	257	31.194	37.986	102.387	1.00	24.60
9891	CD	GLU	B	257	31.497	38.057	103.877	1.00	27.02
9892	OE1	GLU	B	257	32.475	38.734	104.264	1.00	28.68
9893	OE2	GLU	B	257	30.747	37.439	104.663	1.00	29.07
9894	C	GLU	B	257	33.134	38.413	99.120	1.00	22.09
9895	O	GLU	B	257	32.752	39.442	98.571	1.00	21.87
9896	N	ARG	B	258	34.350	37.904	98.945	1.00	22.01
9898	CA	ARG	B	258	35.373	38.561	98.135	1.00	22.01
9900	CB	ARG	B	258	36.723	37.883	98.368	1.00	22.56
9903	CG	ARG	B	258	37.885	38.547	97.664	1.00	24.90
9906	CD	ARG	B	258	39.253	38.114	98.181	1.00	27.91
9909	NE	ARG	B	258	39.582	36.725	97.846	1.00	30.58
9911	CZ	ARG	B	258	39.872	36.275	96.622	1.00	32.32
9912	NH1	ARG	B	258	39.865	37.088	95.568	1.00	33.66
9915	NH2	ARG	B	258	40.165	34.992	96.447	1.00	33.62
9918	C	ARG	B	258	35.031	38.518	96.647	1.00	21.16
9919	O	ARG	B	258	35.134	39.520	95.943	1.00	20.98
9920	N	ILE	B	259	34.616	37.346	96.184	1.00	20.20
9922	CA	ILE	B	259	34.328	37.124	94.773	1.00	19.47
9924	CB	ILE	B	259	34.337	35.588	94.478	1.00	19.65
9926	CG1	ILE	B	259	34.949	35.294	93.099	1.00	20.75
9929	CD1	ILE	B	259	33.988	35.356	91.967	1.00	21.88
9933	CG2	ILE	B	259	32.950	34.966	94.670	1.00	19.57
9937	C	ILE	B	259	33.013	37.815	94.374	1.00	18.39
9938	O	ILE	B	259	32.876	38.295	93.252	1.00	18.01
9939	N	LEU	B	260	32.069	37.885	95.311	1.00	17.19
9941	CA	LEU	B	260	30.824	38.620	95.107	1.00	16.57
9943	CB	LEU	B	260	29.790	38.264	96.180	1.00	16.55
9946	CG	LEU	B	260	29.098	36.910	96.006	1.00	16.74

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9948	CD1	LEU	B	260	28.268	36.577	97.235	1.00	16.89
9952	CD2	LEU	B	260	28.228	36.890	94.750	1.00	16.61
9956	C	LEU	B	260	31.056	40.129	95.094	1.00	15.92
9957	O	LEU	B	260	30.385	40.845	94.360	1.00	15.43
9958	N	ALA	B	261	32.004	40.605	95.902	1.00	15.12
9960	CA	ALA	B	261	32.334	42.028	95.954	1.00	14.57
9962	CB	ALA	B	261	33.229	42.326	97.144	1.00	14.69
9966	C	ALA	B	261	33.013	42.465	94.664	1.00	14.22
9967	O	ALA	B	261	32.779	43.568	94.169	1.00	13.99
9968	N	ARG	B	262	33.858	41.594	94.120	1.00	13.59
9970	CA	ARG	B	262	34.502	41.863	92.844	1.00	13.34
9972	CB	ARG	B	262	35.649	40.877	92.587	1.00	13.63
9975	CG	ARG	B	262	36.893	41.164	93.437	1.00	14.81
9978	CD	ARG	B	262	37.809	42.212	92.837	1.00	16.51
9981	NE	ARG	B	262	38.608	42.922	93.839	1.00	17.95
9983	CZ	ARG	B	262	39.720	42.449	94.406	1.00	19.42
9984	NH1	ARG	B	262	40.370	43.186	95.299	1.00	19.80
9987	NH2	ARG	B	262	40.186	41.244	94.100	1.00	19.98
9990	C	ARG	B	262	33.471	41.829	91.716	1.00	12.56
9991	O	ARG	B	262	33.590	42.584	90.755	1.00	12.44
9992	N	TYR	B	263	32.448	40.984	91.841	1.00	11.71
9994	CA	TYR	B	263	31.390	40.945	90.833	1.00	11.23
9996	CB	TYR	B	263	30.447	39.743	91.010	1.00	11.19
9999	CG	TYR	B	263	29.384	39.722	89.930	1.00	10.32
10000	CD1	TYR	B	263	28.101	40.208	90.178	1.00	10.00
10002	CE1	TYR	B	263	27.133	40.224	89.180	1.00	9.69
10004	CZ	TYR	B	263	27.448	39.766	87.911	1.00	9.66
10005	OH	TYR	B	263	26.488	39.785	86.922	1.00	9.51
10007	CE2	TYR	B	263	28.718	39.293	87.635	1.00	10.00
10009	CD2	TYR	B	263	29.682	39.279	88.643	1.00	9.45
10011	C	TYR	B	263	30.594	42.260	90.833	1.00	11.02
10012	O	TYR	B	263	30.283	42.793	89.770	1.00	10.51
10013	N	GLU	B	264	30.284	42.788	92.017	1.00	10.83
10015	CA	GLU	B	264	29.582	44.075	92.122	1.00	11.08
10017	CB	GLU	B	264	29.341	44.461	93.586	1.00	10.98
10020	CG	GLU	B	264	28.317	43.593	94.290	1.00	12.06
10023	CD	GLU	B	264	26.958	43.640	93.620	1.00	13.73
10024	OE1	GLU	B	264	26.511	42.597	93.091	1.00	15.53
10025	OE2	GLU	B	264	26.347	44.722	93.619	1.00	14.46
10026	C	GLU	B	264	30.337	45.199	91.411	1.00	10.96
10027	O	GLU	B	264	29.731	46.036	90.743	1.00	10.79
10028	N	GLU	B	265	31.657	45.206	91.564	1.00	10.79
10030	CA	GLU	B	265	32.516	46.176	90.893	1.00	10.77
10032	CB	GLU	B	265	33.968	46.003	91.358	1.00	10.86
10035	CG	GLU	B	265	34.229	46.561	92.753	1.00	11.45
10038	CD	GLU	B	265	35.343	45.854	93.513	1.00	12.76
10039	OE1	GLU	B	265	36.118	45.086	92.907	1.00	12.62
10040	OE2	GLU	B	265	35.446	46.076	94.740	1.00	13.93
10041	C	GLU	B	265	32.408	46.045	89.365	1.00	10.27
10042	O	GLU	B	265	32.420	47.046	88.650	1.00	10.26
10043	N	SER	B	266	32.280	44.810	88.881	1.00	9.89
10045	CA	SER	B	266	32.172	44.535	87.446	1.00	9.59

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10047	CB	SER	B	266	32.372	43.037	87.162	1.00	9.78
10050	OG	SER	B	266	31.176	42.300	87.361	1.00	8.72
10052	C	SER	B	266	30.853	44.996	86.805	1.00	9.37
10053	O	SER	B	266	30.792	45.150	85.588	1.00	9.16
10054	N	ILE	B	267	29.810	45.203	87.606	1.00	9.35
10056	CA	ILE	B	267	28.484	45.555	87.070	1.00	9.40
10058	CB	ILE	B	267	27.391	44.633	87.658	1.00	9.40
10060	CG1	ILE	B	267	27.391	44.700	89.190	1.00	9.84
10063	CD1	ILE	B	267	26.089	44.326	89.820	1.00	10.39
10067	CG2	ILE	B	267	27.593	43.206	87.178	1.00	9.93
10071	C	ILE	B	267	28.089	47.021	87.269	1.00	9.15
10072	O	ILE	B	267	26.990	47.416	86.884	1.00	8.98
10073	N	VAL	B	268	28.980	47.825	87.845	1.00	8.94
10075	CA	VAL	B	268	28.699	49.245	88.099	1.00	8.61
10077	CB	VAL	B	268	29.942	49.967	88.689	1.00	8.55
10079	CG1	VAL	B	268	29.786	51.487	88.651	1.00	8.86
10083	CG2	VAL	B	268	30.199	49.494	90.119	1.00	8.39
10087	C	VAL	B	268	28.212	49.970	86.841	1.00	8.43
10088	O	VAL	B	268	27.147	50.603	86.849	1.00	8.13
10089	N	TYR	B	269	28.985	49.874	85.765	1.00	8.14
10091	CA	TYR	B	269	28.632	50.546	84.522	1.00	8.09
10093	CB	TYR	B	269	29.823	50.581	83.552	1.00	8.14
10096	CG	TYR	B	269	31.034	51.385	84.020	1.00	7.97
10097	CD1	TYR	B	269	32.282	51.169	83.448	1.00	7.97
10099	CE1	TYR	B	269	33.392	51.876	83.853	1.00	8.69
10101	CZ	TYR	B	269	33.276	52.829	84.845	1.00	8.98
10102	OH	TYR	B	269	34.392	53.530	85.236	1.00	10.02
10104	CE2	TYR	B	269	32.054	53.068	85.442	1.00	9.30
10106	CD2	TYR	B	269	30.938	52.347	85.031	1.00	8.73
10108	C	TYR	B	269	27.416	49.902	83.849	1.00	8.11
10109	O	TYR	B	269	26.576	50.606	83.295	1.00	8.12
10110	N	SER	B	270	27.312	48.577	83.915	1.00	8.07
10112	CA	SER	B	270	26.209	47.859	83.273	1.00	8.44
10114	CB	SER	B	270	26.425	46.341	83.334	1.00	8.39
10117	OG	SER	B	270	27.394	45.930	82.382	1.00	8.03
10119	C	SER	B	270	24.850	48.225	83.880	1.00	8.66
10120	O	SER	B	270	23.845	48.223	83.178	1.00	8.79
10121	N	ARG	B	271	24.823	48.562	85.168	1.00	8.99
10123	CA	ARG	B	271	23.591	49.019	85.821	1.00	9.35
10125	CB	ARG	B	271	23.836	49.327	87.298	1.00	9.52
10128	CG	ARG	B	271	24.149	48.118	88.171	1.00	11.24
10131	CD	ARG	B	271	24.166	48.446	89.658	1.00	13.36
10134	NE	ARG	B	271	22.805	48.693	90.112	1.00	15.53
10136	CZ	ARG	B	271	21.969	47.752	90.547	1.00	17.08
10137	NH1	ARG	B	271	22.356	46.484	90.651	1.00	17.91
10140	NH2	ARG	B	271	20.735	48.088	90.899	1.00	17.29
10143	C	ARG	B	271	23.037	50.278	85.147	1.00	9.25
10144	O	ARG	B	271	21.842	50.548	85.220	1.00	9.14
10145	N	ARG	B	272	23.911	51.051	84.511	1.00	8.96
10147	CA	ARG	B	272	23.513	52.292	83.854	1.00	8.93
10149	CB	ARG	B	272	24.462	53.403	84.290	1.00	9.05
10152	CG	ARG	B	272	24.433	53.652	85.792	1.00	9.52

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10155	CD	ARG	B	272	25.421	54.698	86.264	1.00	9.84
10158	NE	ARG	B	272	25.143	56.012	85.695	1.00	10.08
10160	CZ	ARG	B	272	25.962	57.055	85.750	1.00	11.39
10161	NH1	ARG	B	272	27.146	56.964	86.344	1.00	11.86
10164	NH2	ARG	B	272	25.596	58.203	85.199	1.00	12.40
10167	C	ARG	B	272	23.445	52.219	82.319	1.00	8.99
10168	O	ARG	B	272	23.198	53.235	81.668	1.00	8.85
10169	N	VAL	B	273	23.617	51.025	81.750	1.00	8.97
10171	CA	VAL	B	273	23.668	50.844	80.294	1.00	9.03
10173	CB	VAL	B	273	25.114	50.512	79.828	1.00	8.94
10175	CG1	VAL	B	273	25.151	50.162	78.344	1.00	8.98
10179	CG2	VAL	B	273	26.054	51.684	80.121	1.00	9.31
10183	C	VAL	B	273	22.717	49.754	79.790	1.00	8.97
10184	O	VAL	B	273	21.940	49.982	78.858	1.00	8.92
10185	N	GLY	B	274	22.803	48.567	80.381	1.00	8.83
10187	CA	GLY	B	274	22.027	47.419	79.940	1.00	8.59
10190	C	GLY	B	274	22.853	46.502	79.056	1.00	8.48
10191	O	GLY	B	274	24.071	46.645	78.980	1.00	8.26
10192	N	ASN	B	275	22.183	45.577	78.373	1.00	8.39
10194	CA	ASN	B	275	22.846	44.590	77.511	1.00	8.59
10196	CB	ASN	B	275	21.861	43.471	77.127	1.00	8.23
10199	CG	ASN	B	275	22.550	42.186	76.684	1.00	8.43
10200	OD1	ASN	B	275	23.770	42.131	76.525	1.00	7.88
10201	ND2	ASN	B	275	21.754	41.133	76.487	1.00	8.29
10204	C	ASN	B	275	23.426	45.230	76.245	1.00	8.62
10205	O	ASN	B	275	22.688	45.783	75.435	1.00	8.42
10206	N	LEU	B	276	24.754	45.171	76.114	1.00	8.77
10208	CA	LEU	B	276	25.479	45.549	74.896	1.00	9.11
10210	CB	LEU	B	276	26.873	46.095	75.252	1.00	9.72
10213	CG	LEU	B	276	27.002	47.380	76.045	1.00	11.32
10215	CD1	LEU	B	276	28.398	47.965	75.830	1.00	12.55
10219	CD2	LEU	B	276	25.945	48.352	75.608	1.00	12.60
10223	C	LEU	B	276	25.710	44.357	73.976	1.00	8.49
10224	O	LEU	B	276	26.508	44.440	73.040	1.00	8.12
10225	N	TYR	B	277	25.013	43.260	74.251	1.00	7.99
10227	CA	TYR	B	277	25.235	41.972	73.601	1.00	7.67
10229	CB	TYR	B	277	24.610	41.951	72.198	1.00	7.72
10232	CG	TYR	B	277	23.090	41.839	72.114	1.00	7.87
10233	CD1	TYR	B	277	22.320	41.283	73.145	1.00	8.24
10235	CE1	TYR	B	277	20.932	41.172	73.026	1.00	8.21
10237	CZ	TYR	B	277	20.307	41.610	71.870	1.00	8.56
10238	OH	TYR	B	277	18.937	41.518	71.724	1.00	6.72
10240	CE2	TYR	B	277	21.056	42.160	70.844	1.00	8.41
10242	CD2	TYR	B	277	22.427	42.266	70.970	1.00	8.52
10244	C	TYR	B	277	26.721	41.549	73.595	1.00	7.35
10245	O	TYR	B	277	27.254	41.223	74.655	1.00	7.21
10246	N	THR	B	278	27.384	41.553	72.430	1.00	7.14
10248	CA	THR	B	278	28.789	41.117	72.327	1.00	6.90
10250	CB	THR	B	278	29.330	41.256	70.873	1.00	6.98
10252	OG1	THR	B	278	29.004	42.546	70.338	1.00	6.34
10254	CG2	THR	B	278	28.664	40.261	69.912	1.00	7.04
10258	C	THR	B	278	29.733	41.877	73.274	1.00	6.89

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10259	O	THR	B	278	30.746	41.336	73.726	1.00	6.77
10260	N	GLY	B	279	29.405	43.131	73.559	1.00	6.64
10262	CA	GLY	B	279	30.263	43.984	74.356	1.00	6.77
10265	C	GLY	B	279	30.092	43.870	75.860	1.00	6.78
10266	O	GLY	B	279	30.931	44.380	76.595	1.00	6.90
10267	N	SER	B	280	29.026	43.210	76.311	1.00	6.47
10269	CA	SER	B	280	28.626	43.214	77.722	1.00	6.52
10271	CB	ASER	B	280	27.362	42.384	77.931	0.65	6.09
10274	OG	ASER	B	280	26.265	42.968	77.270	0.65	5.89
10276	C	SER	B	280	29.707	42.707	78.659	1.00	6.62
10277	O	SER	B	280	29.973	43.331	79.679	1.00	6.68
10278	N	LEU	B	281	30.314	41.571	78.312	1.00	6.80
10280	CA	LEU	B	281	31.413	41.002	79.094	1.00	6.89
10282	CB	LEU	B	281	31.925	39.707	78.447	1.00	6.53
10285	CG	LEU	B	281	33.285	39.170	78.900	1.00	6.97
10287	CD1	LEU	B	281	33.266	38.767	80.378	1.00	7.07
10291	CD2	LEU	B	281	33.722	38.000	78.027	1.00	6.76
10295	C	LEU	B	281	32.558	42.000	79.237	1.00	7.09
10296	O	LEU	B	281	33.117	42.165	80.316	1.00	7.44
10297	N	TYR	B	282	32.887	42.668	78.139	1.00	7.32
10299	CA	TYR	B	282	34.042	43.555	78.082	1.00	7.53
10301	CB	TYR	B	282	34.533	43.668	76.625	1.00	7.57
10304	CG	TYR	B	282	34.897	42.284	76.138	1.00	7.84
10305	CD1	TYR	B	282	36.072	41.683	76.560	1.00	8.20
10307	CE1	TYR	B	282	36.397	40.395	76.185	1.00	8.15
10309	CZ	TYR	B	282	35.532	39.674	75.400	1.00	7.98
10310	OH	TYR	B	282	35.883	38.396	75.043	1.00	7.96
10312	CE2	TYR	B	282	34.334	40.233	74.981	1.00	8.19
10314	CD2	TYR	B	282	34.016	41.532	75.364	1.00	7.52
10316	C	TYR	B	282	33.790	44.900	78.769	1.00	7.76
10317	O	TYR	B	282	34.713	45.475	79.329	1.00	7.67
10318	N	LEU	B	283	32.544	45.367	78.768	1.00	8.08
10320	CA	LEU	B	283	32.149	46.505	79.594	1.00	8.42
10322	CB	LEU	B	283	30.690	46.900	79.332	1.00	8.33
10325	CG	LEU	B	283	30.133	48.062	80.162	1.00	8.65
10327	CD1	LEU	B	283	30.934	49.341	79.924	1.00	8.35
10331	CD2	LEU	B	283	28.662	48.275	79.856	1.00	8.88
10335	C	LEU	B	283	32.337	46.141	81.059	1.00	8.46
10336	O	LEU	B	283	32.785	46.961	81.851	1.00	8.58
10337	N	GLY	B	284	32.004	44.901	81.406	1.00	8.54
10339	CA	GLY	B	284	32.200	44.393	82.751	1.00	8.48
10342	C	GLY	B	284	33.658	44.335	83.165	1.00	8.46
10343	O	GLY	B	284	33.972	44.572	84.327	1.00	8.35
10344	N	LEU	B	285	34.549	44.031	82.219	1.00	8.57
10346	CA	LEU	B	285	35.983	44.055	82.473	1.00	8.42
10348	CB	LEU	B	285	36.762	43.508	81.273	1.00	8.56
10351	CG	LEU	B	285	38.289	43.529	81.396	1.00	8.82
10353	CD1	LEU	B	285	38.758	42.636	82.540	1.00	9.33
10357	CD2	LEU	B	285	38.942	43.113	80.083	1.00	9.48
10361	C	LEU	B	285	36.435	45.483	82.785	1.00	8.41
10362	O	LEU	B	285	37.106	45.715	83.781	1.00	8.20
10363	N	ILE	B	286	36.043	46.430	81.938	1.00	8.29

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10365	CA	ILE	B	286	36.368	47.838	82.144	1.00	8.16
10367	CB	ILE	B	286	35.761	48.726	81.033	1.00	8.31
10369	CG1	ILE	B	286	36.370	48.400	79.660	1.00	8.20
10372	CD1	ILE	B	286	35.552	48.935	78.509	1.00	8.61
10376	CG2	ILE	B	286	36.001	50.198	81.348	1.00	8.39
10380	C	ILE	B	286	35.854	48.309	83.497	1.00	8.02
10381	O	ILE	B	286	36.585	48.948	84.244	1.00	7.82
10382	N	SER	B	287	34.594	47.991	83.799	1.00	7.92
10384	CA	SER	B	287	33.946	48.417	85.042	1.00	7.98
10386	CB	SER	B	287	32.468	48.000	85.042	1.00	8.18
10389	OG	SER	B	287	31.825	48.328	86.260	1.00	7.81
10391	C	SER	B	287	34.676	47.834	86.254	1.00	8.22
10392	O	SER	B	287	34.918	48.530	87.241	1.00	8.13
10393	N	LEU	B	288	35.045	46.561	86.161	1.00	8.50
10395	CA	LEU	B	288	35.794	45.889	87.217	1.00	8.70
10397	CB	LEU	B	288	36.064	44.434	86.839	1.00	8.79
10400	CG	LEU	B	288	37.069	43.665	87.703	1.00	8.95
10402	CD1	LEU	B	288	36.578	43.543	89.152	1.00	9.30
10406	CD2	LEU	B	288	37.306	42.296	87.097	1.00	9.59
10410	C	LEU	B	288	37.118	46.595	87.509	1.00	8.83
10411	O	LEU	B	288	37.412	46.918	88.650	1.00	8.65
10412	N	LEU	B	289	37.913	46.831	86.475	1.00	9.21
10414	CA	LEU	B	289	39.248	47.393	86.665	1.00	9.57
10416	CB	LEU	B	289	40.062	47.313	85.365	1.00	9.80
10419	CG	LEU	B	289	40.217	45.921	84.732	1.00	10.65
10421	CD1	LEU	B	289	41.241	45.956	83.614	1.00	11.22
10425	CD2	LEU	B	289	40.581	44.848	85.753	1.00	12.01
10429	C	LEU	B	289	39.174	48.832	87.170	1.00	9.64
10430	O	LEU	B	289	40.038	49.276	87.924	1.00	9.61
10431	N	GLU	B	290	38.120	49.549	86.789	1.00	9.90
10433	CA	GLU	B	290	38.005	50.967	87.131	1.00	10.24
10435	CB	GLU	B	290	37.312	51.734	85.999	1.00	10.18
10438	CG	GLU	B	290	38.204	51.826	84.771	1.00	10.50
10441	CD	GLU	B	290	37.605	52.576	83.598	1.00	10.02
10442	OE1	GLU	B	290	36.447	53.035	83.670	1.00	10.43
10443	OE2	GLU	B	290	38.319	52.708	82.587	1.00	9.76
10444	C	GLU	B	290	37.328	51.213	88.479	1.00	10.55
10445	O	GLU	B	290	37.486	52.284	89.055	1.00	10.75
10446	N	ASN	B	291	36.610	50.218	89.000	1.00	10.94
10448	CA	ASN	B	291	35.886	50.374	90.263	1.00	11.16
10450	CB	ASN	B	291	34.412	50.006	90.081	1.00	11.20
10453	CG	ASN	B	291	33.670	51.036	89.266	1.00	10.60
10454	OD1	ASN	B	291	33.220	52.048	89.797	1.00	9.38
10455	ND2	ASN	B	291	33.577	50.807	87.960	1.00	10.53
10458	C	ASN	B	291	36.482	49.609	91.433	1.00	11.63
10459	O	ASN	B	291	36.191	49.922	92.582	1.00	11.63
10460	N	ALA	B	292	37.311	48.612	91.142	1.00	12.10
10462	CA	ALA	B	292	38.069	47.911	92.176	1.00	12.58
10464	CB	ALA	B	292	38.734	46.679	91.587	1.00	12.69
10468	C	ALA	B	292	39.118	48.863	92.756	1.00	12.97
10469	O	ALA	B	292	39.579	49.783	92.066	1.00	12.80
10470	N	THR	B	293	39.477	48.658	94.022	1.00	13.42

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10472	CA	THR	B	293	40.509	49.478	94.670	1.00	13.76
10474	CB	THR	B	293	39.960	50.179	95.933	1.00	14.00
10476	OG1	THR	B	293	39.536	49.215	96.905	1.00	14.81
10478	CG2	THR	B	293	38.694	50.974	95.618	1.00	14.63
10482	C	THR	B	293	41.794	48.716	95.015	1.00	13.65
10483	O	THR	B	293	42.852	49.336	95.135	1.00	13.76
10484	N	THR	B	294	41.719	47.392	95.168	1.00	13.30
10486	CA	THR	B	294	42.903	46.608	95.557	1.00	13.11
10488	CB	THR	B	294	42.713	45.960	96.950	1.00	13.20
10490	OG1	THR	B	294	41.591	45.073	96.939	1.00	13.10
10492	CG2	THR	B	294	42.367	47.009	98.014	1.00	13.37
10496	C	THR	B	294	43.338	45.542	94.541	1.00	12.72
10497	O	THR	B	294	44.201	44.718	94.842	1.00	12.37
10498	N	LEU	B	295	42.761	45.554	93.342	1.00	12.34
10500	CA	LEU	B	295	43.333	44.773	92.248	1.00	12.08
10502	CB	LEU	B	295	42.425	44.766	91.017	1.00	12.04
10505	CG	LEU	B	295	41.205	43.845	91.065	1.00	11.36
10507	CD1	LEU	B	295	41.609	42.373	91.222	1.00	11.10
10511	CD2	LEU	B	295	40.357	44.041	89.813	1.00	10.64
10515	C	LEU	B	295	44.685	45.381	91.896	1.00	12.01
10516	O	LEU	B	295	44.883	46.587	92.026	1.00	12.07
10517	N	THR	B	296	45.612	44.539	91.459	1.00	11.99
10519	CA	THR	B	296	46.975	44.972	91.168	1.00	12.09
10521	CB	THR	B	296	47.798	45.016	92.486	1.00	12.22
10523	OG1	THR	B	296	49.059	45.662	92.269	1.00	13.26
10525	CG2	THR	B	296	48.160	43.616	92.969	1.00	12.63
10529	C	THR	B	296	47.634	44.065	90.121	1.00	11.68
10530	O	THR	B	296	47.114	43.000	89.793	1.00	11.32
10531	N	ALA	B	297	48.776	44.499	89.599	1.00	11.44
10533	CA	ALA	B	297	49.486	43.753	88.565	1.00	11.31
10535	CB	ALA	B	297	50.763	44.485	88.166	1.00	11.53
10539	C	ALA	B	297	49.808	42.349	89.066	1.00	10.99
10540	O	ALA	B	297	50.191	42.173	90.220	1.00	10.96
10541	N	GLY	B	298	49.622	41.356	88.202	1.00	10.70
10543	CA	GLY	B	298	49.882	39.970	88.540	1.00	10.67
10546	C	GLY	B	298	48.617	39.213	88.906	1.00	10.46
10547	O	GLY	B	298	48.615	37.979	88.920	1.00	10.49
10548	N	ASN	B	299	47.537	39.940	89.190	1.00	10.09
10550	CA	ASN	B	299	46.267	39.312	89.540	1.00	9.92
10552	CB	ASN	B	299	45.272	40.345	90.074	1.00	9.81
10555	CG	ASN	B	299	45.612	40.832	91.480	1.00	9.81
10556	OD1	ASN	B	299	44.929	41.699	92.013	1.00	8.40
10557	ND2	ASN	B	299	46.661	40.277	92.081	1.00	9.67
10560	C	ASN	B	299	45.656	38.588	88.346	1.00	9.90
10561	O	ASN	B	299	45.878	38.968	87.196	1.00	9.78
10562	N	GLN	B	300	44.881	37.549	88.637	1.00	9.93
10564	CA	GLN	B	300	44.281	36.697	87.628	1.00	10.14
10566	CB	GLN	B	300	44.487	35.224	87.994	1.00	10.33
10569	CG	GLN	B	300	45.942	34.839	88.297	1.00	11.22
10572	CD	GLN	B	300	46.828	34.902	87.069	1.00	11.91
10573	OE1	GLN	B	300	46.589	34.192	86.097	1.00	12.61
10574	NE2	GLN	B	300	47.850	35.755	87.107	1.00	12.60

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10577	C	GLN	B	300	42.791	37.001	87.520	1.00	10.07
10578	O	GLN	B	300	42.064	36.949	88.509	1.00	10.00
10579	N	ILE	B	301	42.351	37.324	86.307	1.00	9.95
10581	CA	ILE	B	301	40.956	37.618	86.013	1.00	9.82
10583	CB	ILE	B	301	40.844	38.971	85.264	1.00	9.96
10585	CG1	ILE	B	301	41.716	40.058	85.918	1.00	10.31
10588	CD1	ILE	B	301	41.265	40.496	87.301	1.00	11.11
10592	CG2	ILE	B	301	39.393	39.413	85.162	1.00	10.03
10596	C	ILE	B	301	40.392	36.509	85.128	1.00	9.59
10597	O	ILE	B	301	40.918	36.259	84.046	1.00	9.25
10598	N	GLY	B	302	39.330	35.848	85.583	1.00	9.40
10600	CA	GLY	B	302	38.606	34.887	84.769	1.00	9.46
10603	C	GLY	B	302	37.485	35.575	84.011	1.00	9.41
10604	O	GLY	B	302	36.825	36.464	84.546	1.00	9.85
10605	N	LEU	B	303	37.276	35.167	82.766	1.00	9.07
10607	CA	LEU	B	303	36.279	35.774	81.901	1.00	8.95
10609	CB	LEU	B	303	36.949	36.514	80.739	1.00	9.50
10612	CG	LEU	B	303	37.663	37.825	81.091	1.00	10.11
10614	CD1	LEU	B	303	39.134	37.574	81.356	1.00	10.34
10618	CD2	LEU	B	303	37.481	38.870	79.984	1.00	10.86
10622	C	LEU	B	303	35.370	34.686	81.360	1.00	8.57
10623	O	LEU	B	303	35.839	33.721	80.754	1.00	8.55
10624	N	PHE	B	304	34.073	34.836	81.593	1.00	8.08
10626	CA	PHE	B	304	33.085	33.936	81.030	1.00	7.82
10628	CB	PHE	B	304	32.115	33.445	82.100	1.00	7.60
10631	CG	PHE	B	304	30.958	32.681	81.542	1.00	7.28
10632	CD1	PHE	B	304	29.673	33.208	81.574	1.00	7.17
10634	CE1	PHE	B	304	28.604	32.495	81.046	1.00	6.96
10636	CZ	PHE	B	304	28.821	31.255	80.460	1.00	6.67
10638	CE2	PHE	B	304	30.099	30.730	80.416	1.00	6.91
10640	CD2	PHE	B	304	31.158	31.441	80.949	1.00	6.85
10642	C	PHE	B	304	32.309	34.654	79.931	1.00	7.77
10643	O	PHE	B	304	31.554	35.585	80.207	1.00	7.58
10644	N	SER	B	305	32.506	34.215	78.690	1.00	7.71
10646	CA	SER	B	305	31.731	34.698	77.553	1.00	7.63
10648	CB	SER	B	305	32.635	34.891	76.342	1.00	7.57
10651	OG	SER	B	305	31.920	35.487	75.273	1.00	7.26
10653	C	SER	B	305	30.616	33.713	77.209	1.00	7.72
10654	O	SER	B	305	30.833	32.505	77.170	1.00	7.62
10655	N	TYR	B	306	29.419	34.242	76.990	1.00	7.94
10657	CA	TYR	B	306	28.277	33.448	76.564	1.00	8.04
10659	CB	TYR	B	306	27.218	33.380	77.674	1.00	7.99
10662	CG	TYR	B	306	26.006	32.532	77.322	1.00	8.04
10663	CD1	TYR	B	306	24.823	33.122	76.876	1.00	8.05
10665	CE1	TYR	B	306	23.708	32.354	76.545	1.00	7.08
10667	CZ	TYR	B	306	23.766	30.979	76.664	1.00	7.96
10668	OH	TYR	B	306	22.662	30.222	76.337	1.00	7.85
10670	CE2	TYR	B	306	24.932	30.364	77.099	1.00	8.28
10672	CD2	TYR	B	306	26.045	31.144	77.426	1.00	8.41
10674	C	TYR	B	306	27.660	34.070	75.325	1.00	8.18
10675	O	TYR	B	306	27.620	35.289	75.181	1.00	8.43
10676	N	GLY	B	307	27.178	33.210	74.440	1.00	7.95

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10678	CA	GLY	B	307	26.350	33.606	73.322	1.00	7.95
10681	C	GLY	B	307	25.236	32.584	73.197	1.00	7.86
10682	O	GLY	B	307	25.502	31.383	73.185	1.00	7.81
10683	N	SER	B	308	23.992	33.046	73.122	1.00	7.74
10685	CA	SER	B	308	22.845	32.157	72.942	1.00	7.75
10687	CB	SER	B	308	21.541	32.959	72.952	1.00	7.91
10690	OG	SER	B	308	21.143	33.290	74.272	1.00	6.86
10692	C	SER	B	308	22.964	31.360	71.637	1.00	8.10
10693	O	SER	B	308	23.571	31.825	70.666	1.00	8.23
10694	N	GLY	B	309	22.408	30.151	71.619	1.00	8.33
10696	CA	GLY	B	309	22.468	29.313	70.435	1.00	8.54
10699	C	GLY	B	309	22.934	27.873	70.600	1.00	8.72
10700	O	GLY	B	309	22.453	27.026	69.848	1.00	9.10
10701	N	ALA	B	310	23.860	27.550	71.507	1.00	8.68
10703	CA	ALA	B	310	24.628	28.475	72.342	1.00	8.65
10705	CB	ALA	B	310	24.087	28.460	73.762	1.00	8.78
10709	C	ALA	B	310	26.116	28.105	72.356	1.00	8.73
10710	O	ALA	B	310	26.478	26.927	72.255	1.00	8.36
10711	N	VAL	B	311	26.969	29.121	72.471	1.00	8.77
10713	CA	VAL	B	311	28.414	28.945	72.582	1.00	9.03
10715	CB	VAL	B	311	29.128	29.463	71.312	1.00	9.32
10717	CG1	VAL	B	311	30.653	29.311	71.426	1.00	9.40
10721	CG2	VAL	B	311	28.607	28.729	70.083	1.00	9.55
10725	C	VAL	B	311	28.932	29.687	73.815	1.00	9.21
10726	O	VAL	B	311	28.533	30.822	74.082	1.00	9.22
10727	N	ALA	B	312	29.810	29.044	74.577	1.00	9.04
10729	CA	ALA	B	312	30.395	29.665	75.759	1.00	9.26
10731	CB	ALA	B	312	29.721	29.137	77.019	1.00	9.15
10735	C	ALA	B	312	31.896	29.426	75.821	1.00	9.44
10736	O	ALA	B	312	32.413	28.501	75.197	1.00	9.47
10737	N	GLU	B	313	32.589	30.262	76.586	1.00	9.49
10739	CA	GLU	B	313	34.022	30.122	76.776	1.00	9.77
10741	CB	GLU	B	313	34.781	30.776	75.617	1.00	9.90
10744	CG	GLU	B	313	36.283	30.503	75.623	1.00	11.38
10747	CD	GLU	B	313	36.969	30.864	74.311	1.00	12.61
10748	OE1	GLU	B	313	36.280	31.010	73.281	1.00	15.57
10749	OE2	GLU	B	313	38.206	30.993	74.305	1.00	13.36
10750	C	GLU	B	313	34.472	30.723	78.108	1.00	9.75
10751	O	GLU	B	313	33.991	31.778	78.516	1.00	9.60
10752	N	PHE	B	314	35.373	30.022	78.790	1.00	9.50
10754	CA	PHE	B	314	36.051	30.548	79.966	1.00	9.43
10756	CB	PHE	B	314	35.821	29.649	81.181	1.00	9.53
10759	CG	PHE	B	314	36.267	30.262	82.479	1.00	9.86
10760	CD1	PHE	B	314	35.409	31.063	83.216	1.00	10.20
10762	CE1	PHE	B	314	35.825	31.640	84.415	1.00	10.63
10764	CZ	PHE	B	314	37.101	31.417	84.883	1.00	10.35
10766	CE2	PHE	B	314	37.969	30.625	84.162	1.00	11.01
10768	CD2	PHE	B	314	37.550	30.050	82.957	1.00	11.06
10770	C	PHE	B	314	37.540	30.655	79.655	1.00	9.36
10771	O	PHE	B	314	38.144	29.717	79.141	1.00	8.56
10772	N	PHE	B	315	38.121	31.811	79.950	1.00	9.48
10774	CA	PHE	B	315	39.539	32.053	79.712	1.00	9.75

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10776	CB	PHE	B	315	39.775	32.527	78.270	1.00	9.70
10779	CG	PHE	B	315	39.054	33.808	77.919	1.00	10.09
10780	CD1	PHE	B	315	39.736	35.019	77.886	1.00	10.68
10782	CE1	PHE	B	315	39.078	36.201	77.564	1.00	10.85
10784	CZ	PHE	B	315	37.720	36.180	77.264	1.00	10.84
10786	CE2	PHE	B	315	37.030	34.982	77.287	1.00	10.85
10788	CD2	PHE	B	315	37.698	33.799	77.617	1.00	10.37
10790	C	PHE	B	315	40.077	33.075	80.707	1.00	9.92
10791	O	PHE	B	315	39.316	33.781	81.363	1.00	10.02
10792	N	THR	B	316	41.396	33.154	80.810	1.00	10.03
10794	CA	THR	B	316	42.028	33.930	81.862	1.00	10.28
10796	CB	THR	B	316	42.806	32.985	82.794	1.00	10.46
10798	OG1	THR	B	316	41.881	32.095	83.435	1.00	10.48
10800	CG2	THR	B	316	43.449	33.745	83.948	1.00	10.51
10804	C	THR	B	316	42.949	34.992	81.297	1.00	10.32
10805	O	THR	B	316	43.600	34.780	80.282	1.00	10.55
10806	N	GLY	B	317	42.977	36.144	81.957	1.00	10.33
10808	CA	GLY	B	317	43.947	37.183	81.672	1.00	10.25
10811	C	GLY	B	317	44.677	37.578	82.939	1.00	10.08
10812	O	GLY	B	317	44.163	37.395	84.041	1.00	10.03
10813	N	GLU	B	318	45.887	38.104	82.785	1.00	9.99
10815	CA	GLU	B	318	46.665	38.606	83.906	1.00	9.90
10817	CB	GLU	B	318	48.042	37.938	83.953	1.00	9.90
10820	CG	GLU	B	318	48.883	38.381	85.143	1.00	9.97
10823	CD	GLU	B	318	50.151	37.568	85.310	1.00	10.49
10824	OE1	GLU	B	318	51.235	38.183	85.426	1.00	10.14
10825	OE2	GLU	B	318	50.056	36.325	85.323	1.00	10.10
10826	C	GLU	B	318	46.826	40.113	83.766	1.00	9.85
10827	O	GLU	B	318	47.167	40.594	82.698	1.00	9.86
10828	N	LEU	B	319	46.587	40.855	84.843	1.00	9.99
10830	CA	LEU	B	319	46.809	42.299	84.830	1.00	10.27
10832	CB	LEU	B	319	46.222	42.955	86.084	1.00	10.12
10835	CG	LEU	B	319	44.691	42.947	86.168	1.00	10.48
10837	CD1	LEU	B	319	44.217	43.417	87.548	1.00	10.28
10841	CD2	LEU	B	319	44.074	43.794	85.066	1.00	10.29
10845	C	LEU	B	319	48.309	42.616	84.698	1.00	10.41
10846	O	LEU	B	319	49.139	42.070	85.419	1.00	10.27
10847	N	VAL	B	320	48.631	43.505	83.768	1.00	10.75
10849	CA	VAL	B	320	50.007	43.828	83.408	1.00	11.23
10851	CB	VAL	B	320	50.082	44.223	81.911	1.00	11.47
10853	CG1	VAL	B	320	51.453	44.782	81.534	1.00	12.40
10857	CG2	VAL	B	320	49.731	43.014	81.039	1.00	11.82
10861	C	VAL	B	320	50.503	44.974	84.284	1.00	11.28
10862	O	VAL	B	320	49.720	45.830	84.683	1.00	11.34
10863	N	ALA	B	321	51.800	44.989	84.578	1.00	11.28
10865	CA	ALA	B	321	52.406	46.086	85.331	1.00	11.21
10867	CB	ALA	B	321	53.906	45.863	85.476	1.00	11.40
10871	C	ALA	B	321	52.126	47.427	84.652	1.00	11.10
10872	O	ALA	B	321	52.298	47.570	83.443	1.00	10.84
10873	N	GLY	B	322	51.667	48.399	85.437	1.00	11.32
10875	CA	GLY	B	322	51.389	49.731	84.935	1.00	11.26
10878	C	GLY	B	322	49.987	49.917	84.387	1.00	11.39

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10879	O	GLY	B	322	49.644	51.027	83.993	1.00	11.41
10880	N	TYR	B	323	49.172	48.858	84.381	1.00	11.50
10882	CA	TYR	B	323	47.818	48.913	83.802	1.00	11.55
10884	CB	TYR	B	323	47.088	47.560	83.931	1.00	11.46
10887	CG	TYR	B	323	46.376	47.353	85.256	1.00	11.15
10888	CD1	TYR	B	323	45.025	47.673	85.405	1.00	10.98
10890	CE1	TYR	B	323	44.372	47.501	86.629	1.00	10.95
10892	CZ	TYR	B	323	45.071	46.999	87.711	1.00	10.34
10893	OH	TYR	B	323	44.448	46.820	88.924	1.00	9.24
10895	CE2	TYR	B	323	46.411	46.678	87.584	1.00	10.56
10897	CD2	TYR	B	323	47.056	46.861	86.363	1.00	10.56
10899	C	TYR	B	323	46.947	50.012	84.405	1.00	11.80
10900	O	TYR	B	323	46.089	50.566	83.714	1.00	11.82
10901	N	GLN	B	324	47.154	50.306	85.687	1.00	12.05
10903	CA	GLN	B	324	46.369	51.319	86.399	1.00	12.67
10905	CB	GLN	B	324	46.698	51.311	87.901	1.00	12.71
10908	CG	GLN	B	324	46.159	50.075	88.632	1.00	12.91
10911	CD	GLN	B	324	46.549	49.995	90.108	1.00	13.52
10912	OE1	GLN	B	324	47.270	50.856	90.621	1.00	13.51
10913	NE2	GLN	B	324	46.074	48.951	90.789	1.00	11.56
10916	C	GLN	B	324	46.539	52.730	85.827	1.00	13.12
10917	O	GLN	B	324	45.626	53.548	85.931	1.00	12.98
10918	N	ASN	B	325	47.696	53.012	85.230	1.00	13.76
10920	CA	ASN	B	325	47.920	54.287	84.530	1.00	14.65
10922	CB	ASN	B	325	49.406	54.465	84.187	1.00	14.60
10925	CG	ASN	B	325	50.270	54.692	85.414	1.00	14.64
10926	OD1	ASN	B	325	49.832	55.299	86.386	1.00	14.06
10927	ND2	ASN	B	325	51.510	54.210	85.365	1.00	13.91
10930	C	ASN	B	325	47.105	54.440	83.239	1.00	15.39
10931	O	ASN	B	325	47.009	55.537	82.693	1.00	15.58
10932	N	HIS	B	326	46.542	53.343	82.742	1.00	16.27
10934	CA	HIS	B	326	45.810	53.350	81.478	1.00	17.13
10936	CB	HIS	B	326	46.309	52.213	80.599	1.00	17.21
10939	CG	HIS	B	326	47.773	52.286	80.319	1.00	17.01
10940	ND1	HIS	B	326	48.292	53.019	79.276	1.00	17.40
10942	CE1	HIS	B	326	49.607	52.913	79.280	1.00	18.32
10944	NE2	HIS	B	326	49.961	52.149	80.298	1.00	18.38
10946	CD2	HIS	B	326	48.830	51.750	80.967	1.00	17.77
10948	C	HIS	B	326	44.309	53.237	81.672	1.00	17.92
10949	O	HIS	B	326	43.569	53.056	80.705	1.00	18.15
10950	N	LEU	B	327	43.868	53.346	82.923	1.00	18.77
10952	CA	LEU	B	327	42.450	53.329	83.246	1.00	19.23
10954	CB	LEU	B	327	42.229	52.907	84.699	1.00	19.36
10957	CG	LEU	B	327	42.715	51.503	85.058	1.00	19.44
10959	CD1	LEU	B	327	42.460	51.236	86.529	1.00	20.03
10963	CD2	LEU	B	327	42.059	50.436	84.181	1.00	19.68
10967	C	LEU	B	327	41.869	54.711	83.016	1.00	19.68
10968	O	LEU	B	327	42.586	55.714	83.054	1.00	19.85
10969	N	GLN	B	328	40.558	54.753	82.805	1.00	19.92
10971	CA	GLN	B	328	39.881	55.956	82.342	1.00	20.27
10973	CB	GLN	B	328	39.688	55.875	80.825	1.00	20.63
10976	CG	GLN	B	328	40.814	56.464	79.991	1.00	22.15

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10979	CD	GLN	B	328	40.374	56.764	78.562	1.00	24.10
10980	OE1	GLN	B	328	39.263	56.392	78.157	1.00	25.37
10981	NE2	GLN	B	328	41.241	57.433	77.793	1.00	23.77
10984	C	GLN	B	328	38.526	56.116	83.022	1.00	20.05
10985	O	GLN	B	328	37.524	56.368	82.354	1.00	19.77
10986	N	LYS	B	329	38.502	55.976	84.347	1.00	19.72
10988	CA	LYS	B	329	37.259	56.072	85.115	1.00	19.68
10990	CB	LYS	B	329	37.530	55.899	86.611	1.00	19.77
10993	CG	LYS	B	329	36.277	55.639	87.435	1.00	20.23
10996	CD	LYS	B	329	36.519	55.913	88.906	1.00	21.51
10999	CE	LYS	B	329	35.656	55.039	89.781	1.00	22.41
11002	NZ	LYS	B	329	36.072	55.129	91.205	1.00	23.61
11006	C	LYS	B	329	36.533	57.397	84.892	1.00	19.63
11007	O	LYS	B	329	35.317	57.418	84.701	1.00	19.12
11008	N	GLU	B	330	37.285	58.494	84.933	1.00	19.55
11010	CA	GLU	B	330	36.713	59.833	84.794	1.00	19.83
11012	CB	GLU	B	330	37.780	60.893	85.100	1.00	20.28
11015	CG	GLU	B	330	37.474	62.303	84.616	1.00	22.37
11018	CD	GLU	B	330	38.633	63.250	84.862	1.00	24.86
11019	OE1	GLU	B	330	39.109	63.308	86.017	1.00	27.03
11020	OE2	GLU	B	330	39.081	63.919	83.899	1.00	27.23
11021	C	GLU	B	330	36.105	60.044	83.407	1.00	19.11
11022	O	GLU	B	330	35.031	60.613	83.285	1.00	19.45
11023	N	THR	B	331	36.795	59.579	82.370	1.00	18.47
11025	CA	THR	B	331	36.300	59.685	81.000	1.00	18.03
11027	CB	THR	B	331	37.352	59.158	80.009	1.00	18.07
11029	OG1	THR	B	331	38.534	59.969	80.075	1.00	18.47
11031	CG2	THR	B	331	36.884	59.303	78.569	1.00	18.27
11035	C	THR	B	331	34.992	58.905	80.841	1.00	17.47
11036	O	THR	B	331	34.076	59.349	80.156	1.00	17.18
11037	N	HIS	B	332	34.909	57.756	81.500	1.00	16.75
11039	CA	HIS	B	332	33.762	56.869	81.360	1.00	16.28
11041	CB	HIS	B	332	34.164	55.452	81.760	1.00	16.09
11044	CG	HIS	B	332	35.111	54.817	80.789	1.00	14.98
11045	ND1	HIS	B	332	35.833	53.683	81.080	1.00	13.68
11047	CE1	HIS	B	332	36.566	53.348	80.033	1.00	14.64
11049	NE2	HIS	B	332	36.359	54.235	79.077	1.00	14.91
11051	CD2	HIS	B	332	35.457	55.168	79.526	1.00	15.06
11053	C	HIS	B	332	32.537	57.362	82.129	1.00	16.07
11054	O	HIS	B	332	31.429	57.333	81.604	1.00	15.85
11055	N	LEU	B	333	32.734	57.843	83.350	1.00	15.90
11057	CA	LEU	B	333	31.632	58.410	84.120	1.00	16.07
11059	CB	LEU	B	333	32.043	58.675	85.571	1.00	16.27
11062	CG	LEU	B	333	32.150	57.447	86.484	1.00	16.83
11064	CD1	LEU	B	333	32.671	57.863	87.856	1.00	17.10
11068	CD2	LEU	B	333	30.817	56.732	86.617	1.00	16.94
11072	C	LEU	B	333	31.099	59.698	83.472	1.00	15.92
11073	O	LEU	B	333	29.910	59.982	83.559	1.00	15.74
11074	N	ALA	B	334	31.979	60.456	82.819	1.00	15.69
11076	CA	ALA	B	334	31.588	61.652	82.072	1.00	15.54
11078	CB	ALA	B	334	32.822	62.429	81.612	1.00	15.66
11082	C	ALA	B	334	30.722	61.291	80.865	1.00	15.16

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11083	O	ALA	B	334	29.765	61.988	80.560	1.00	14.91
11084	N	LEU	B	335	31.067	60.208	80.180	1.00	14.79
11086	CA	LEU	B	335	30.277	59.733	79.047	1.00	14.69
11088	CB	LEU	B	335	30.939	58.515	78.408	1.00	14.76
11091	CG	LEU	B	335	30.201	57.857	77.243	1.00	15.26
11093	CD1	LEU	B	335	30.196	58.771	76.030	1.00	15.87
11097	CD2	LEU	B	335	30.849	56.519	76.922	1.00	15.88
11101	C	LEU	B	335	28.858	59.372	79.483	1.00	14.40
11102	O	LEU	B	335	27.894	59.698	78.795	1.00	14.15
11103	N	LEU	B	336	28.741	58.707	80.631	1.00	14.05
11105	CA	LEU	B	336	27.443	58.288	81.149	1.00	14.11
11107	CB	LEU	B	336	27.619	57.245	82.257	1.00	14.12
11110	CG	LEU	B	336	28.312	55.948	81.818	1.00	14.19
11112	CD1	LEU	B	336	28.616	55.070	83.030	1.00	14.30
11116	CD2	LEU	B	336	27.466	55.188	80.792	1.00	14.15
11120	C	LEU	B	336	26.648	59.488	81.655	1.00	14.14
11121	O	LEU	B	336	25.460	59.630	81.347	1.00	13.93
11122	N	ASP	B	337	27.316	60.367	82.399	1.00	14.27
11124	CA	ASP	B	337	26.667	61.532	83.010	1.00	14.58
11126	CB	ASP	B	337	27.629	62.238	83.983	1.00	15.00
11129	CG	ASP	B	337	27.795	61.494	85.295	1.00	15.71
11130	OD1	ASP	B	337	28.893	61.558	85.884	1.00	17.33
11131	OD2	ASP	B	337	26.883	60.835	85.828	1.00	17.68
11132	C	ASP	B	337	26.164	62.545	81.978	1.00	14.37
11133	O	ASP	B	337	25.165	63.218	82.206	1.00	14.11
11134	N	ASN	B	338	26.854	62.642	80.845	1.00	14.23
11136	CA	ASN	B	338	26.540	63.651	79.835	1.00	14.33
11138	CB	ASN	B	338	27.790	63.996	79.015	1.00	14.85
11141	CG	ASN	B	338	28.759	64.909	79.772	1.00	17.05
11142	OD1	ASN	B	338	28.359	65.659	80.670	1.00	20.29
11143	ND2	ASN	B	338	30.037	64.852	79.404	1.00	19.22
11146	C	ASN	B	338	25.384	63.254	78.910	1.00	13.44
11147	O	ASN	B	338	24.949	64.054	78.082	1.00	13.44
11148	N	ARG	B	339	24.876	62.034	79.065	1.00	12.30
11150	CA	ARG	B	339	23.697	61.594	78.323	1.00	11.61
11152	CB	ARG	B	339	23.446	60.097	78.523	1.00	11.32
11155	CG	ARG	B	339	24.606	59.192	78.137	1.00	10.86
11158	CD	ARG	B	339	24.343	57.721	78.393	1.00	10.19
11161	NE	ARG	B	339	24.177	57.436	79.815	1.00	8.74
11163	CZ	ARG	B	339	23.827	56.253	80.315	1.00	7.48
11164	NH1	ARG	B	339	23.598	55.220	79.517	1.00	5.57
11167	NH2	ARG	B	339	23.698	56.113	81.630	1.00	7.50
11170	C	ARG	B	339	22.447	62.347	78.761	1.00	11.24
11171	O	ARG	B	339	22.357	62.831	79.890	1.00	11.15
11172	N	THR	B	340	21.481	62.418	77.855	1.00	10.68
11174	CA	THR	B	340	20.192	63.034	78.120	1.00	10.42
11176	CB	THR	B	340	19.749	63.841	76.903	1.00	10.52
11178	OG1	THR	B	340	20.736	64.836	76.611	1.00	9.95
11180	CG2	THR	B	340	18.467	64.627	77.197	1.00	11.00
11184	C	THR	B	340	19.165	61.957	78.420	1.00	10.01
11185	O	THR	B	340	18.967	61.041	77.628	1.00	9.79
11186	N	GLU	B	341	18.523	62.065	79.574	1.00	9.45

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11188	CA	GLU	B	341	17.428	61.176	79.916	1.00	9.20
11190	CB	GLU	B	341	17.063	61.324	81.389	1.00	9.01
11193	CG	GLU	B	341	16.157	60.226	81.919	1.00	9.16
11196	CD	GLU	B	341	15.612	60.550	83.295	1.00	9.02
11197	OE1	GLU	B	341	14.546	60.006	83.655	1.00	9.03
11198	OE2	GLU	B	341	16.233	61.374	83.998	1.00	7.47
11199	C	GLU	B	341	16.217	61.497	79.047	1.00	8.95
11200	O	GLU	B	341	15.935	62.668	78.762	1.00	8.22
11201	N	LEU	B	342	15.513	60.446	78.635	1.00	8.86
11203	CA	LEU	B	342	14.274	60.568	77.881	1.00	8.98
11205	CB	LEU	B	342	14.300	59.667	76.641	1.00	8.94
11208	CG	LEU	B	342	15.437	59.828	75.623	1.00	8.96
11210	CD1	LEU	B	342	15.405	58.693	74.617	1.00	8.88
11214	CD2	LEU	B	342	15.364	61.165	74.908	1.00	8.66
11218	C	LEU	B	342	13.125	60.132	78.781	1.00	8.98
11219	O	LEU	B	342	13.287	59.244	79.627	1.00	9.12
11220	N	SER	B	343	11.964	60.754	78.603	1.00	9.16
11222	CA	SER	B	343	10.744	60.270	79.235	1.00	9.05
11224	CB	SER	B	343	9.618	61.288	79.106	1.00	9.13
11227	OG	SER	B	343	9.175	61.380	77.770	1.00	8.54
11229	C	SER	B	343	10.367	58.977	78.528	1.00	9.18
11230	O	SER	B	343	10.869	58.696	77.438	1.00	9.00
11231	N	ILE	B	344	9.489	58.189	79.129	1.00	9.29
11233	CA	ILE	B	344	9.124	56.917	78.522	1.00	9.73
11235	CB	ILE	B	344	8.264	56.053	79.468	1.00	9.81
11237	CG1	ILE	B	344	9.051	55.708	80.741	1.00	10.18
11240	CD1	ILE	B	344	10.390	54.979	80.502	1.00	10.70
11244	CG2	ILE	B	344	7.801	54.767	78.760	1.00	10.09
11248	C	ILE	B	344	8.441	57.156	77.176	1.00	9.76
11249	O	ILE	B	344	8.692	56.423	76.237	1.00	9.79
11250	N	ALA	B	345	7.618	58.199	77.072	1.00	9.86
11252	CA	ALA	B	345	6.952	58.521	75.810	1.00	9.91
11254	CB	ALA	B	345	5.944	59.643	76.001	1.00	10.10
11258	C	ALA	B	345	7.966	58.893	74.725	1.00	10.00
11259	O	ALA	B	345	7.839	58.457	73.578	1.00	9.82
11260	N	GLU	B	346	8.968	59.689	75.090	1.00	10.02
11262	CA	GLU	B	346	10.037	60.058	74.158	1.00	10.20
11264	CB	GLU	B	346	10.998	61.062	74.798	1.00	10.37
11267	CG	GLU	B	346	10.446	62.476	74.897	1.00	11.02
11270	CD	GLU	B	346	11.320	63.407	75.725	1.00	12.36
11271	OE1	GLU	B	346	11.062	64.631	75.709	1.00	12.10
11272	OE2	GLU	B	346	12.263	62.925	76.393	1.00	12.68
11273	C	GLU	B	346	10.800	58.809	73.723	1.00	10.06
11274	O	GLU	B	346	11.132	58.650	72.556	1.00	10.08
11275	N	TYR	B	347	11.050	57.919	74.677	1.00	9.82
11277	CA	TYR	B	347	11.751	56.665	74.423	1.00	9.70
11279	CB	TYR	B	347	12.035	55.951	75.749	1.00	9.72
11282	CG	TYR	B	347	12.048	54.436	75.705	1.00	9.50
11283	CD1	TYR	B	347	10.987	53.694	76.212	1.00	8.99
11285	CE1	TYR	B	347	11.007	52.307	76.194	1.00	8.24
11287	CZ	TYR	B	347	12.108	51.649	75.681	1.00	8.67
11288	OH	TYR	B	347	12.142	50.276	75.660	1.00	7.76

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11290	CE2	TYR	B	347	13.179	52.364	75.184	1.00	8.99
11292	CD2	TYR	B	347	13.145	53.749	75.207	1.00	9.88
11294	C	TYR	B	347	10.959	55.764	73.483	1.00	9.76
11295	O	TYR	B	347	11.526	55.183	72.572	1.00	8.87
11296	N	GLU	B	348	9.651	55.664	73.699	1.00	10.00
11298	CA	GLU	B	348	8.802	54.808	72.874	1.00	10.55
11300	CB	GLU	B	348	7.389	54.718	73.454	1.00	10.69
11303	CG	GLU	B	348	7.311	53.871	74.711	1.00	11.67
11306	CD	GLU	B	348	5.889	53.552	75.132	1.00	13.62
11307	OE1	GLU	B	348	4.951	54.276	74.730	1.00	15.63
11308	OE2	GLU	B	348	5.710	52.570	75.870	1.00	13.66
11309	C	GLU	B	348	8.759	55.285	71.424	1.00	10.83
11310	O	GLU	B	348	8.742	54.470	70.509	1.00	10.67
11311	N	ALA	B	349	8.764	56.602	71.228	1.00	11.02
11313	CA	ALA	B	349	8.812	57.193	69.893	1.00	11.40
11315	CB	ALA	B	349	8.563	58.698	69.972	1.00	11.42
11319	C	ALA	B	349	10.154	56.910	69.209	1.00	11.57
11320	O	ALA	B	349	10.190	56.495	68.053	1.00	11.54
11321	N	MSE	B	350	11.252	57.129	69.927	1.00	11.95
11323	CA	MSE	B	350	12.587	56.821	69.409	1.00	12.09
11325	CB	MSE	B	350	13.663	57.217	70.423	1.00	12.03
11328	CG	MSE	B	350	15.085	57.087	69.900	1.00	12.10
11331	SE	MSE	B	350	16.436	57.770	71.113	1.00	13.04
11332	CE	MSE	B	350	16.184	59.696	70.854	1.00	12.21
11336	C	MSE	B	350	12.720	55.332	69.071	1.00	12.20
11337	O	MSE	B	350	13.240	54.976	68.017	1.00	12.36
11338	N	PHE	B	351	12.230	54.483	69.972	1.00	12.37
11340	CA	PHE	B	351	12.328	53.029	69.852	1.00	12.49
11342	CB	PHE	B	351	11.750	52.362	71.108	1.00	12.28
11345	CG	PHE	B	351	11.927	50.868	71.140	1.00	12.01
11346	CD1	PHE	B	351	11.057	50.031	70.447	1.00	11.28
11348	CE1	PHE	B	351	11.227	48.654	70.468	1.00	11.12
11350	CZ	PHE	B	351	12.262	48.099	71.185	1.00	11.10
11352	CE2	PHE	B	351	13.131	48.915	71.887	1.00	11.90
11354	CD2	PHE	B	351	12.960	50.297	71.864	1.00	11.87
11356	C	PHE	B	351	11.597	52.484	68.627	1.00	13.09
11357	O	PHE	B	351	12.132	51.645	67.898	1.00	13.05
11358	N	ALA	B	352	10.369	52.955	68.425	1.00	13.62
11360	CA	ALA	B	352	9.491	52.445	67.378	1.00	14.47
11362	CB	ALA	B	352	8.042	52.830	67.671	1.00	14.45
11366	C	ALA	B	352	9.881	52.936	65.991	1.00	15.20
11367	O	ALA	B	352	9.490	52.329	64.995	1.00	15.48
11368	N	GLU	B	353	10.639	54.029	65.919	1.00	16.19
11370	CA	GLU	B	353	11.013	54.606	64.631	1.00	17.09
11372	CB	GLU	B	353	11.842	55.884	64.801	1.00	17.36
11375	CG	GLU	B	353	11.970	56.698	63.518	1.00	18.49
11378	CD	GLU	B	353	12.588	58.072	63.725	1.00	20.21
11379	OE1	GLU	B	353	12.501	58.903	62.792	1.00	22.36
11380	OE2	GLU	B	353	13.165	58.328	64.804	1.00	20.88
11381	C	GLU	B	353	11.779	53.588	63.790	1.00	17.43
11382	O	GLU	B	353	12.602	52.827	64.302	1.00	16.88
11383	N	THR	B	354	11.470	53.580	62.498	1.00	18.19

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11385	CA	THR	B	354	12.065	52.665	61.539	1.00	18.88
11387	CB	THR	B	354	10.977	51.765	60.911	1.00	19.26
11389	OG1	THR	B	354	9.926	52.573	60.359	1.00	19.89
11391	CG2	THR	B	354	10.280	50.919	61.978	1.00	19.66
11395	C	THR	B	354	12.778	53.463	60.451	1.00	19.00
11396	O	THR	B	354	12.411	54.601	60.154	1.00	19.34
11397	N	LEU	B	355	13.825	52.867	59.897	1.00	19.13
11399	CA	LEU	B	355	14.575	53.444	58.791	1.00	19.02
11401	CB	LEU	B	355	16.074	53.456	59.112	1.00	19.22
11404	CG	LEU	B	355	17.057	53.885	58.021	1.00	19.75
11406	CD1	LEU	B	355	16.872	55.348	57.709	1.00	20.55
11410	CD2	LEU	B	355	18.491	53.610	58.458	1.00	20.02
11414	C	LEU	B	355	14.300	52.576	57.577	1.00	18.55
11415	O	LEU	B	355	14.691	51.407	57.545	1.00	18.57
11416	N	ASP	B	356	13.588	53.140	56.606	1.00	17.99
11418	CA	ASP	B	356	13.376	52.480	55.332	1.00	17.65
11420	CB	ASP	B	356	12.046	52.917	54.707	1.00	17.85
11423	CG	ASP	B	356	11.619	52.024	53.544	1.00	18.42
11424	OD1	ASP	B	356	12.467	51.283	52.999	1.00	17.69
11425	OD2	ASP	B	356	10.446	51.992	53.106	1.00	20.33
11426	C	ASP	B	356	14.554	52.836	54.428	1.00	17.05
11427	O	ASP	B	356	14.610	53.931	53.864	1.00	16.95
11428	N	THR	B	357	15.494	51.900	54.305	1.00	16.42
11430	CA	THR	B	357	16.702	52.101	53.503	1.00	15.93
11432	CB	THR	B	357	17.798	51.080	53.887	1.00	15.93
11434	OG1	THR	B	357	17.286	49.740	53.810	1.00	15.83
11436	CG2	THR	B	357	18.214	51.249	55.336	1.00	16.00
11440	C	THR	B	357	16.456	52.046	51.989	1.00	15.54
11441	O	THR	B	357	17.355	52.345	51.217	1.00	14.91
11442	N	ASP	B	358	15.252	51.660	51.572	1.00	15.35
11444	CA	ASP	B	358	14.860	51.737	50.161	1.00	15.59
11446	CB	ASP	B	358	13.758	50.716	49.850	1.00	15.74
11449	CG	ASP	B	358	14.283	49.292	49.785	1.00	16.61
11450	OD1	ASP	B	358	15.506	49.108	49.563	1.00	17.22
11451	OD2	ASP	B	358	13.549	48.296	49.949	1.00	17.15
11452	C	ASP	B	358	14.409	53.145	49.744	1.00	15.48
11453	O	ASP	B	358	14.120	53.379	48.569	1.00	15.12
11454	N	ILE	B	359	14.370	54.071	50.703	1.00	15.32
11456	CA	ILE	B	359	14.000	55.462	50.455	1.00	15.41
11458	CB	ILE	B	359	12.851	55.890	51.401	1.00	15.60
11460	CG1	ILE	B	359	11.617	55.017	51.141	1.00	16.35
11463	CD1	ILE	B	359	10.384	55.403	51.938	1.00	17.78
11467	CG2	ILE	B	359	12.521	57.390	51.214	1.00	15.96
11471	C	ILE	B	359	15.212	56.365	50.650	1.00	14.95
11472	O	ILE	B	359	15.777	56.430	51.745	1.00	14.64
11473	N	ASP	B	360	15.607	57.050	49.581	1.00	14.56
11475	CA	ASP	B	360	16.681	58.035	49.639	1.00	14.42
11477	CB	ASP	B	360	17.019	58.554	48.239	1.00	14.36
11480	CG	ASP	B	360	17.728	57.516	47.379	1.00	14.74
11481	OD1	ASP	B	360	17.999	57.811	46.195	1.00	14.42
11482	OD2	ASP	B	360	18.055	56.383	47.795	1.00	14.37
11483	C	ASP	B	360	16.276	59.196	50.553	1.00	14.32

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11484	O	ASP	B	360	15.209	59.788	50.387	1.00	13.96
11485	N	GLN	B	361	17.134	59.509	51.517	1.00	14.17
11487	CA	GLN	B	361	16.824	60.506	52.540	1.00	14.32
11489	CB	GLN	B	361	15.877	59.896	53.581	1.00	14.41
11492	CG	GLN	B	361	16.436	58.642	54.279	1.00	15.13
11495	CD	GLN	B	361	15.370	57.832	55.008	1.00	16.45
11496	OE1	GLN	B	361	14.836	58.274	56.025	1.00	17.74
11497	NE2	GLN	B	361	15.065	56.649	54.492	1.00	17.76
11500	C	GLN	B	361	18.079	61.010	53.243	1.00	14.13
11501	O	GLN	B	361	19.140	60.384	53.175	1.00	14.32
11502	N	THR	B	362	17.945	62.146	53.921	1.00	13.74
11504	CA	THR	B	362	18.947	62.622	54.864	1.00	13.49
11506	CB	THR	B	362	19.278	64.110	54.630	1.00	13.57
11508	OG1	THR	B	362	18.088	64.900	54.742	1.00	13.40
11510	CG2	THR	B	362	19.763	64.353	53.198	1.00	13.84
11514	C	THR	B	362	18.423	62.429	56.283	1.00	13.44
11515	O	THR	B	362	17.210	62.468	56.526	1.00	13.00
11516	N	LEU	B	363	19.351	62.205	57.208	1.00	13.20
11518	CA	LEU	B	363	19.050	62.092	58.626	1.00	13.20
11520	CB	LEU	B	363	19.522	60.741	59.162	1.00	13.16
11523	CG	ALEU	B	363	18.766	59.500	58.666	0.65	12.86
11525	CD1	ALEU	B	363	19.211	59.086	57.262	0.65	12.75
11529	CD2	ALEU	B	363	18.942	58.339	59.639	0.65	12.75
11533	C	LEU	B	363	19.756	63.232	59.350	1.00	13.39
11534	O	LEU	B	363	20.832	63.666	58.931	1.00	13.20
11535	N	GLU	B	364	19.136	63.719	60.421	1.00	13.53
11537	CA	GLU	B	364	19.674	64.823	61.207	1.00	13.88
11539	CB	GLU	B	364	18.611	65.912	61.371	1.00	14.21
11542	CG	GLU	B	364	19.117	67.169	62.056	1.00	14.98
11545	CD	GLU	B	364	18.143	68.332	61.957	1.00	16.33
11546	OE1	GLU	B	364	16.919	68.101	61.794	1.00	15.82
11547	OE2	GLU	B	364	18.615	69.484	62.046	1.00	16.94
11548	C	GLU	B	364	20.111	64.296	62.573	1.00	13.74
11549	O	GLU	B	364	19.288	63.818	63.351	1.00	13.49
11550	N	ASP	B	365	21.411	64.377	62.843	1.00	13.35
11552	CA	ASP	B	365	21.987	63.891	64.093	1.00	13.46
11554	CB	ASP	B	365	22.141	62.363	64.039	1.00	13.29
11557	CG	ASP	B	365	22.368	61.732	65.409	1.00	13.47
11558	OD1	ASP	B	365	22.897	62.400	66.320	1.00	12.97
11559	OD2	ASP	B	365	22.050	60.552	65.668	1.00	13.18
11560	C	ASP	B	365	23.347	64.554	64.284	1.00	13.53
11561	O	ASP	B	365	24.183	64.522	63.384	1.00	13.41
11562	N	GLU	B	366	23.577	65.136	65.456	1.00	13.68
11564	CA	GLU	B	366	24.826	65.860	65.709	1.00	14.09
11566	CB	GLU	B	366	24.602	66.926	66.793	1.00	14.74
11569	CG	GLU	B	366	23.671	68.058	66.354	1.00	17.25
11572	CD	GLU	B	366	23.964	68.554	64.940	1.00	20.82
11573	OE1	GLU	B	366	25.076	69.085	64.710	1.00	23.21
11574	OE2	GLU	B	366	23.089	68.398	64.051	1.00	23.46
11575	C	GLU	B	366	26.012	64.953	66.078	1.00	13.37
11576	O	GLU	B	366	27.162	65.401	66.071	1.00	13.09
11577	N	LEU	B	367	25.737	63.684	66.380	1.00	12.58

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11579	CA	LEU	B	367	26.779	62.749	66.800	1.00	12.06
11581	CB	LEU	B	367	26.152	61.463	67.353	1.00	12.12
11584	CG	LEU	B	367	27.113	60.407	67.915	1.00	12.42
11586	CD1	LEU	B	367	27.876	60.948	69.112	1.00	13.19
11590	CD2	LEU	B	367	26.360	59.133	68.290	1.00	12.59
11594	C	LEU	B	367	27.718	62.405	65.646	1.00	11.46
11595	O	LEU	B	367	27.271	62.093	64.547	1.00	11.04
11596	N	LYS	B	368	29.022	62.456	65.904	1.00	10.93
11598	CA	LYS	B	368	30.010	62.027	64.921	1.00	10.70
11600	CB	LYS	B	368	31.431	62.236	65.443	1.00	10.71
11603	CG	LYS	B	368	32.509	62.197	64.370	1.00	11.24
11606	CD	LYS	B	368	33.875	62.468	64.994	1.00	11.42
11609	CE	LYS	B	368	34.974	62.497	63.966	1.00	11.16
11612	NZ	LYS	B	368	36.316	62.456	64.603	1.00	11.46
11616	C	LYS	B	368	29.787	60.553	64.588	1.00	10.25
11617	O	LYS	B	368	29.490	59.750	65.471	1.00	9.62
11618	N	TYR	B	369	29.904	60.229	63.302	1.00	10.05
11620	CA	TYR	B	369	29.729	58.868	62.774	1.00	10.10
11622	CB	TYR	B	369	30.653	57.859	63.477	1.00	10.21
11625	CG	TYR	B	369	32.125	58.219	63.420	1.00	10.85
11626	CD1	TYR	B	369	32.889	58.307	64.585	1.00	11.50
11628	CE1	TYR	B	369	34.234	58.632	64.537	1.00	11.51
11630	CZ	TYR	B	369	34.834	58.873	63.321	1.00	11.71
11631	OH	TYR	B	369	36.169	59.198	63.274	1.00	13.04
11633	CE2	TYR	B	369	34.103	58.793	62.152	1.00	11.79
11635	CD2	TYR	B	369	32.756	58.461	62.206	1.00	11.05
11637	C	TYR	B	369	28.279	58.359	62.777	1.00	9.87
11638	O	TYR	B	369	28.037	57.183	62.489	1.00	9.44
11639	N	SER	B	370	27.319	59.233	63.079	1.00	9.72
11641	CA	SER	B	370	25.908	58.910	62.876	1.00	9.85
11643	CB	SER	B	370	24.989	59.905	63.602	1.00	9.99
11646	OG	SER	B	370	25.220	61.238	63.201	1.00	9.45
11648	C	SER	B	370	25.602	58.893	61.385	1.00	10.03
11649	O	SER	B	370	26.346	59.456	60.579	1.00	10.10
11650	N	ILE	B	371	24.510	58.235	61.021	1.00	10.28
11652	CA	ILE	B	371	24.082	58.155	59.629	1.00	10.27
11654	CB	ILE	B	371	22.924	57.137	59.454	1.00	10.13
11656	CG1	ILE	B	371	23.315	55.755	59.980	1.00	9.89
11659	CD1	ILE	B	371	22.140	54.883	60.313	1.00	9.38
11663	CG2	ILE	B	371	22.528	57.026	57.982	1.00	10.55
11667	C	ILE	B	371	23.622	59.537	59.179	1.00	10.40
11668	O	ILE	B	371	22.709	60.109	59.777	1.00	10.47
11669	N	SER	B	372	24.269	60.057	58.138	1.00	10.37
11671	CA	SER	B	372	23.928	61.340	57.521	1.00	10.72
11673	CB	SER	B	372	25.210	62.047	57.063	1.00	10.69
11676	OG	SER	B	372	25.960	61.220	56.189	1.00	10.82
11678	C	SER	B	372	22.969	61.209	56.323	1.00	10.91
11679	O	SER	B	372	22.193	62.126	56.048	1.00	11.12
11680	N	ALA	B	373	23.032	60.089	55.607	1.00	10.97
11682	CA	ALA	B	373	22.185	59.881	54.427	1.00	11.30
11684	CB	ALA	B	373	22.717	60.710	53.244	1.00	11.23
11688	C	ALA	B	373	22.054	58.415	54.004	1.00	11.59

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11689	O	ALA	B	373	22.896	57.581	54.339	1.00	11.84
11690	N	ILE	B	374	20.975	58.123	53.281	1.00	11.72
11692	CA	ILE	B	374	20.789	56.872	52.550	1.00	11.93
11694	CB	ILE	B	374	19.510	56.130	53.019	1.00	12.18
11696	CG1	ILE	B	374	19.485	55.945	54.543	1.00	12.53
11699	CD1	ILE	B	374	20.529	55.009	55.087	1.00	13.42
11703	CG2	ILE	B	374	19.375	54.788	52.295	1.00	12.25
11707	C	ILE	B	374	20.645	57.214	51.065	1.00	11.83
11708	O	ILE	B	374	19.832	58.063	50.704	1.00	11.77
11709	N	ASN	B	375	21.446	56.569	50.218	1.00	11.82
11711	CA	ASN	B	375	21.369	56.721	48.761	1.00	11.71
11713	CB	ASN	B	375	22.489	57.613	48.232	1.00	11.99
11716	CG	ASN	B	375	22.465	58.996	48.817	1.00	13.40
11717	OD1	ASN	B	375	23.199	59.292	49.765	1.00	16.17
11718	ND2	ASN	B	375	21.633	59.865	48.251	1.00	14.40
11721	C	ASN	B	375	21.516	55.357	48.108	1.00	11.32
11722	O	ASN	B	375	22.553	54.718	48.251	1.00	10.98
11723	N	ASN	B	376	20.493	54.924	47.377	1.00	10.94
11725	CA	ASN	B	376	20.491	53.610	46.744	1.00	10.89
11727	CB	ASN	B	376	21.491	53.608	45.581	1.00	10.79
11730	CG	ASN	B	376	21.255	52.471	44.605	1.00	10.95
11731	OD1	ASN	B	376	20.116	52.089	44.338	1.00	10.69
11732	ND2	ASN	B	376	22.337	51.917	44.079	1.00	9.65
11735	C	ASN	B	376	20.791	52.480	47.749	1.00	10.66
11736	O	ASN	B	376	21.508	51.533	47.433	1.00	10.56
11737	N	THR	B	377	20.226	52.621	48.953	1.00	10.48
11739	CA	THR	B	377	20.414	51.732	50.121	1.00	10.44
11741	CB	THR	B	377	20.190	50.230	49.796	1.00	10.42
11743	OG1	THR	B	377	21.307	49.708	49.062	1.00	9.67
11745	CG2	THR	B	377	18.961	50.000	48.910	1.00	10.33
11749	C	THR	B	377	21.737	51.875	50.889	1.00	10.57
11750	O	THR	B	377	21.884	51.291	51.964	1.00	10.34
11751	N	VAL	B	378	22.677	52.649	50.353	1.00	10.71
11753	CA	VAL	B	378	23.988	52.829	50.967	1.00	11.00
11755	CB	VAL	B	378	25.051	53.187	49.909	1.00	11.03
11757	CG1	VAL	B	378	26.416	53.423	50.562	1.00	11.00
11761	CG2	VAL	B	378	25.139	52.080	48.851	1.00	11.52
11765	C	VAL	B	378	23.967	53.920	52.040	1.00	11.06
11766	O	VAL	B	378	23.514	55.033	51.792	1.00	11.30
11767	N	ARG	B	379	24.477	53.589	53.222	1.00	11.19
11769	CA	ARG	B	379	24.560	54.527	54.334	1.00	11.40
11771	CB	ARG	B	379	24.609	53.779	55.669	1.00	11.23
11774	CG	ARG	B	379	23.323	53.073	56.039	1.00	11.32
11777	CD	ARG	B	379	23.515	51.907	56.980	1.00	11.16
11780	NE	ARG	B	379	22.319	51.068	57.081	1.00	10.96
11782	CZ	ARG	B	379	21.563	50.924	58.174	1.00	11.65
11783	NH1	ARG	B	379	21.852	51.560	59.304	1.00	11.54
11786	NH2	ARG	B	379	20.504	50.125	58.140	1.00	11.82
11789	C	ARG	B	379	25.807	55.392	54.215	1.00	11.75
11790	O	ARG	B	379	26.894	54.888	53.925	1.00	11.88
11791	N	SER	B	380	25.636	56.690	54.434	1.00	11.98
11793	CA	SER	B	380	26.748	57.615	54.605	1.00	12.68

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11795	CB	SER	B	380	26.558	58.861	53.740	1.00	12.84
11798	OG	SER	B	380	26.702	58.548	52.369	1.00	13.53
11800	C	SER	B	380	26.800	58.007	56.076	1.00	13.02
11801	O	SER	B	380	25.762	58.087	56.735	1.00	13.05
11802	N	TYR	B	381	28.007	58.229	56.587	1.00	13.54
11804	CA	TYR	B	381	28.214	58.643	57.970	1.00	14.00
11806	CB	TYR	B	381	29.032	57.583	58.715	1.00	13.66
11809	CG	TYR	B	381	28.379	56.219	58.691	1.00	12.45
11810	CD1	TYR	B	381	27.465	55.850	59.669	1.00	11.45
11812	CE1	TYR	B	381	26.853	54.609	59.650	1.00	10.51
11814	CZ	TYR	B	381	27.140	53.719	58.634	1.00	9.82
11815	OH	TYR	B	381	26.522	52.493	58.617	1.00	8.76
11817	CE2	TYR	B	381	28.040	54.059	57.642	1.00	10.75
11819	CD2	TYR	B	381	28.653	55.308	57.672	1.00	11.09
11821	C	TYR	B	381	28.921	59.998	57.996	1.00	15.25
11822	O	TYR	B	381	29.795	60.261	57.169	1.00	14.80
11823	N	ARG	B	382	28.554	60.856	58.942	1.00	16.86
11825	CA	ARG	B	382	29.159	62.188	59.008	1.00	18.63
11827	CB	ARG	B	382	28.236	63.223	59.664	1.00	18.86
11830	CG	ARG	B	382	27.522	62.776	60.917	1.00	19.83
11833	CD	ARG	B	382	26.739	63.892	61.600	1.00	21.14
11836	NE	ARG	B	382	25.698	64.481	60.752	1.00	21.52
11838	CZ	ARG	B	382	24.529	63.908	60.433	1.00	22.44
11839	NH1	ARG	B	382	23.669	64.566	59.660	1.00	21.88
11842	NH2	ARG	B	382	24.201	62.691	60.876	1.00	21.78
11845	C	ARG	B	382	30.516	62.129	59.707	1.00	19.76
11846	O	ARG	B	382	30.681	61.431	60.705	1.00	19.63
11847	N	ASN	B	383	31.480	62.859	59.151	1.00	21.37
11849	CA	ASN	B	383	32.865	62.851	59.624	1.00	22.70
11851	CB	ASN	B	383	33.830	63.068	58.448	1.00	23.01
11854	CG	ASN	B	383	33.830	61.910	57.472	1.00	24.08
11855	OD1	ASN	B	383	34.305	60.816	57.787	1.00	25.76
11856	ND2	ASN	B	383	33.291	62.140	56.280	1.00	25.55
11859	C	ASN	B	383	33.147	63.910	60.685	1.00	23.37
11860	O	ASN	B	383	34.212	63.891	61.293	1.00	23.83
11861	N	ALA	B	384	32.211	64.837	60.884	1.00	24.20
11863	CA	ALA	B	384	32.358	65.910	61.869	1.00	24.72
11865	CB	ALA	B	384	32.183	67.269	61.196	1.00	24.93
11869	C	ALA	B	384	31.350	65.744	63.003	1.00	24.96
11870	O	ALA	B	384	30.169	65.479	62.761	1.00	25.48
11871	O20	hmg	X	1	31.868	38.489	46.772	1.00	15.99
11872	C26	hmg	X	1	30.626	38.392	46.633	1.00	15.92
11873	O19	hmg	X	1	29.883	38.193	47.613	1.00	18.35
11874	C25	hmg	X	1	29.940	38.529	45.287	1.00	14.18
11877	C23	hmg	X	1	30.762	38.109	44.064	1.00	13.23
11878	C24	hmg	X	1	29.898	38.350	42.827	1.00	12.51
11882	O18	hmg	X	1	31.037	36.709	44.114	1.00	12.37
11884	C22	hmg	X	1	32.091	38.869	44.040	1.00	11.82
11887	C21	hmg	X	1	32.696	39.018	42.669	1.00	11.05
11888	O16	hmg	X	1	33.313	38.085	42.190	1.00	9.37
11889	S1	hmg	X	1	32.545	40.457	41.827	1.00	10.73
11890	C20	hmg	X	1	33.185	40.192	40.201	1.00	9.89

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11893	C19	hmg	X	1	32.189	39.424	39.338	1.00	10.32
11896	N7	hmg	X	1	30.871	40.030	39.359	1.00	9.93
11898	C18	hmg	X	1	29.736	39.331	39.344	1.00	10.11
11899	O15	hmg	X	1	29.695	38.111	39.243	1.00	9.92
11900	C17	hmg	X	1	28.484	40.167	39.503	1.00	10.48
11903	C16	hmg	X	1	27.223	39.436	39.053	1.00	11.03
11906	N6	hmg	X	1	27.148	39.324	37.610	1.00	12.15
11908	C15	hmg	X	1	26.796	40.345	36.823	1.00	13.34
11909	O14	hmg	X	1	26.531	41.458	37.250	1.00	12.82
11910	C14	hmg	X	1	26.684	40.090	35.342	1.00	14.71
11912	O13	hmg	X	1	26.319	38.734	35.126	1.00	15.28
11914	C11	hmg	X	1	27.965	40.423	34.562	1.00	16.13
11915	C12	hmg	X	1	29.089	39.441	34.879	1.00	16.05
11919	C13	hmg	X	1	28.411	41.857	34.869	1.00	16.20
11923	C10	hmg	X	1	27.618	40.346	33.076	1.00	17.27
11926	O12	hmg	X	1	26.622	41.318	32.760	1.00	18.86
11927	P3	hmg	X	1	26.208	41.601	31.233	1.00	19.72
11928	O21	hmg	X	1	25.807	40.292	30.612	1.00	20.64
11929	O11	hmg	X	1	25.254	42.767	31.204	1.00	20.68
11930	O10	hmg	X	1	27.604	42.121	30.626	1.00	23.32
11931	P2	hmg	X	1	28.155	41.680	29.184	1.00	24.56
11932	O8	hmg	X	1	26.996	41.798	28.224	1.00	25.81
11933	O9	hmg	X	1	29.401	42.483	28.926	1.00	25.22
11934	O7	hmg	X	1	28.543	40.122	29.493	1.00	26.01
11935	C9	hmg	X	1	29.867	39.564	29.368	1.00	25.84
11938	C8	hmg	X	1	30.039	39.551	27.861	1.00	26.40
11940	O6	hmg	X	1	29.639	38.328	27.221	1.00	25.32
11941	C2	hmg	X	1	30.272	38.248	25.940	1.00	25.49
11943	C27	hmg	X	1	31.124	39.492	25.870	1.00	26.22
11945	O5	hmg	X	1	31.762	40.050	24.736	1.00	26.95
11947	C1	hmg	X	1	31.191	40.120	27.146	1.00	26.45
11949	O4	hmg	X	1	32.557	40.136	27.378	1.00	27.24
11950	P1	hmg	X	1	33.564	40.594	28.544	1.00	27.29
11951	O3	hmg	X	1	33.667	42.084	28.324	1.00	28.06
11952	O2	hmg	X	1	32.960	40.186	29.868	1.00	26.87
11953	O1	hmg	X	1	34.799	39.816	28.164	1.00	26.70
11954	N1	hmg	X	1	29.209	38.073	24.946	1.00	24.42
11955	C3	hmg	X	1	29.154	37.087	24.086	1.00	23.85
11956	N5	hmg	X	1	30.113	36.034	23.879	1.00	23.94
11957	C6	hmg	X	1	29.866	35.127	22.916	1.00	24.50
11959	N2	hmg	X	1	28.758	35.189	22.148	1.00	24.47
11960	C4	hmg	X	1	27.955	37.205	23.300	1.00	24.15
11961	N4	hmg	X	1	27.311	38.289	23.759	1.00	24.47
11962	C7	hmg	X	1	28.084	38.801	24.771	1.00	24.37
11964	C5	hmg	X	1	27.811	36.149	22.277	1.00	24.50
11965	N3	hmg	X	1	26.727	36.171	21.488	1.00	24.92
11968	O20	hmg	C	2	23.707	35.925	73.506	1.00	10.15
11969	C26	hmg	C	2	22.774	36.641	73.076	1.00	11.05
11970	O19	hmg	C	2	22.782	37.084	71.910	1.00	13.42
11971	C25	hmg	C	2	21.562	36.997	73.912	1.00	10.04
11974	C23	hmg	C	2	21.775	37.152	75.420	1.00	9.18
11975	C24	hmg	C	2	20.404	37.467	76.009	1.00	9.46

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
11979	O18	hmg	C	2	22.634	38.262	75.711	1.00	9.55
11981	C22	hmg	C	2	22.392	35.881	76.006	1.00	8.43
11984	C21	hmg	C	2	22.075	35.682	77.465	1.00	8.13
11985	O16	hmg	C	2	22.686	36.321	78.307	1.00	7.08
11986	S1	hmg	C	2	20.905	34.583	77.929	1.00	8.74
11987	C20	hmg	C	2	20.632	34.802	79.666	1.00	8.25
11990	C19	hmg	C	2	19.904	36.111	79.956	1.00	8.97
11993	N7	hmg	C	2	18.666	36.203	79.208	1.00	9.40
11995	C18	hmg	C	2	18.153	37.348	78.760	1.00	10.53
11996	O15	hmg	C	2	18.631	38.450	79.004	1.00	10.76
11997	C17	hmg	C	2	16.940	37.177	77.871	1.00	10.92
12000	C16	hmg	C	2	16.104	38.447	77.748	1.00	10.64
12003	N6	hmg	C	2	15.371	38.763	78.958	1.00	11.19
12005	C15	hmg	C	2	14.282	38.084	79.326	1.00	10.99
12006	O14	hmg	C	2	13.863	37.130	78.694	1.00	10.16
12007	C14	hmg	C	2	13.532	38.542	80.548	1.00	11.79
12009	O13	hmg	C	2	13.727	39.934	80.792	1.00	10.64
12011	C11	hmg	C	2	13.915	37.742	81.804	1.00	13.34
12012	C12	hmg	C	2	15.333	38.081	82.272	1.00	12.94
12016	C13	hmg	C	2	13.775	36.242	81.543	1.00	12.79
12020	C10	hmg	C	2	12.918	38.124	82.893	1.00	14.51
12023	O12	hmg	C	2	11.594	37.770	82.471	1.00	17.05
12024	P3	hmg	C	2	10.375	37.838	83.521	1.00	17.65
12025	O21	hmg	C	2	10.254	39.262	83.967	1.00	17.96
12026	O11	hmg	C	2	9.195	37.088	82.968	1.00	18.32
12027	O10	hmg	C	2	11.005	36.885	84.644	1.00	20.11
12028	P2	hmg	C	2	10.826	37.019	86.230	1.00	19.88
12029	O8	hmg	C	2	9.422	37.460	86.553	1.00	20.92
12030	O9	hmg	C	2	11.321	35.693	86.735	1.00	21.45
12031	O7	hmg	C	2	11.935	38.176	86.495	1.00	21.21
12032	C9	hmg	C	2	13.226	37.926	87.091	1.00	20.86
12035	C8	hmg	C	2	12.818	38.049	88.539	1.00	20.88
12037	O6	hmg	C	2	12.864	39.320	89.172	1.00	19.87
12038	C2	hmg	C	2	12.673	39.054	90.564	1.00	19.41
12040	C27	hmg	C	2	12.633	37.556	90.706	1.00	20.36
12042	O5	hmg	C	2	12.200	36.783	91.809	1.00	20.14
12044	C1	hmg	C	2	13.042	36.967	89.487	1.00	20.50
12046	O4	hmg	C	2	14.247	36.404	89.829	1.00	20.31
12047	P1	hmg	C	2	15.173	35.228	89.274	1.00	21.14
12048	O3	hmg	C	2	15.739	35.754	87.971	1.00	21.13
12049	O2	hmg	C	2	16.202	35.149	90.368	1.00	21.23
12050	O1	hmg	C	2	14.259	34.033	89.164	1.00	20.10
12051	N1	hmg	C	2	11.460	39.798	90.890	1.00	18.09
12052	C3	hmg	C	2	11.445	40.736	91.787	1.00	16.85
12053	N5	hmg	C	2	12.546	41.120	92.627	1.00	16.04
12054	C6	hmg	C	2	12.324	42.088	93.516	1.00	16.36
12056	N2	hmg	C	2	11.121	42.682	93.619	1.00	15.98
12057	C4	hmg	C	2	10.133	41.324	91.853	1.00	16.34
12058	N4	hmg	C	2	9.399	40.690	90.923	1.00	17.10
12059	C7	hmg	C	2	10.225	39.769	90.329	1.00	17.27
12061	C5	hmg	C	2	10.026	42.379	92.880	1.00	16.77
12062	N3	hmg	C	2	8.864	43.034	93.075	1.00	17.55

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
12065	OW0	HOH	X	3	38.424	46.015	96.138	1.00	10.91
12068	OW0	HOH	X	5	23.251	55.339	76.560	1.00	4.08
12071	OW0	HOH	X	8	8.607	58.942	82.102	1.00	8.82
12074	OW0	HOH	X	9	28.153	37.875	67.300	1.00	6.53
12077	OW0	HOH	X	10	29.857	37.117	75.955	1.00	6.04
12080	OW0	HOH	X	12	18.714	47.130	80.539	1.00	5.61
12083	OW0	HOH	X	13	22.167	29.796	61.737	1.00	5.44
12086	OW0	HOH	X	14	35.886	24.893	39.446	1.00	5.82
12089	OW0	HOH	X	15	31.134	29.774	37.855	1.00	11.32
12092	OW0	HOH	X	16	18.207	57.905	86.339	1.00	13.38
12095	OW0	HOH	X	17	19.197	26.203	61.374	1.00	10.08
12098	OW0	HOH	X	18	32.294	28.739	40.816	1.00	8.00
12101	OW0	HOH	X	19	40.758	59.928	70.661	1.00	5.94
12104	OW0	HOH	X	20	27.102	27.680	35.812	1.00	7.78
12107	OW0	HOH	X	22	13.260	29.188	46.179	1.00	9.93
12110	OW0	HOH	X	23	25.961	44.934	80.308	1.00	4.83
12113	OW0	HOH	X	24	17.574	22.600	31.472	1.00	11.37
12116	OW0	HOH	X	25	31.119	35.560	54.121	1.00	6.56
12119	OW0	HOH	X	26	49.629	52.391	70.506	1.00	7.54
12122	OW0	HOH	X	27	18.136	24.543	63.420	1.00	8.23
12125	OW0	HOH	X	28	45.770	51.153	77.296	1.00	7.32
12128	OW0	HOH	X	29	20.232	44.769	81.353	1.00	9.18
12131	OW0	HOH	X	30	10.646	25.324	67.959	1.00	9.42
12134	OW0	HOH	X	31	21.576	33.121	69.085	1.00	4.38
12137	OW0	HOH	X	32	23.620	21.384	41.494	1.00	9.96
12140	OW0	HOH	X	33	23.199	48.315	63.532	1.00	8.16
12143	OW0	HOH	X	34	13.305	58.192	82.153	1.00	8.26
12146	OW0	HOH	X	35	28.352	52.691	54.390	1.00	8.76
12149	OW0	HOH	X	37	16.373	27.720	62.787	1.00	9.42
12152	OW0	HOH	X	38	18.128	42.902	69.553	1.00	9.00
12155	OW0	HOH	X	39	27.041	59.275	74.181	1.00	10.46
12158	OW0	HOH	X	40	45.418	31.732	86.234	1.00	12.59
12161	OW0	HOH	X	41	49.530	47.467	89.556	1.00	12.58
12164	OW0	HOH	X	42	27.323	50.916	56.489	1.00	9.07
12167	OW0	HOH	X	43	31.421	38.816	72.462	1.00	5.42
12170	OW0	HOH	X	44	11.707	25.714	45.953	1.00	10.55
12173	OW0	HOH	X	47	8.842	65.271	74.374	1.00	8.31
12176	OW0	HOH	X	48	10.604	40.418	65.647	1.00	14.02
12179	OW0	HOH	X	50	41.412	53.142	55.819	1.00	10.46
12182	OW0	HOH	X	51	38.606	26.839	87.079	1.00	8.76
12185	OW0	HOH	X	52	42.630	48.242	91.920	1.00	8.51
12188	OW0	HOH	X	53	30.872	53.521	53.638	1.00	7.68
12191	OW0	HOH	X	55	8.230	45.101	79.110	1.00	8.72
12194	OW0	HOH	X	56	40.466	29.216	39.727	1.00	10.68
12197	OW0	HOH	X	60	31.984	45.645	95.661	1.00	8.86
12200	OW0	HOH	X	61	22.439	35.778	46.479	1.00	10.36
12203	OW0	HOH	X	62	46.801	29.437	36.733	1.00	12.66
12206	OW0	HOH	X	64	20.665	48.925	63.292	1.00	14.68
12209	OW0	HOH	X	65	46.804	17.179	40.622	1.00	9.71
12212	OW0	HOH	X	66	20.703	48.056	55.668	1.00	12.67
12215	OW0	HOH	X	67	20.977	34.620	19.495	1.00	85.42
12218	OW0	HOH	X	68	41.058	9.513	57.018	1.00	21.38

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
12221	OW0	HOH	X	69	29.544	46.730	83.884	1.00	7.67
12224	OW0	HOH	X	70	53.708	37.543	43.427	1.00	12.84
12227	OW0	HOH	X	71	18.522	43.932	46.172	1.00	11.07
12230	OW0	HOH	X	72	23.482	52.940	88.958	1.00	10.46
12233	OW0	HOH	X	73	16.985	53.110	66.824	1.00	8.48
12236	OW0	HOH	X	74	43.483	58.490	60.558	1.00	12.33
12239	OW0	HOH	X	75	28.947	31.305	37.415	1.00	9.97
12242	OW0	HOH	X	76	14.239	53.156	66.409	1.00	8.05
12245	OW0	HOH	X	77	23.165	16.499	45.164	1.00	7.44
12248	OW0	HOH	X	78	10.025	22.809	40.120	1.00	13.26
12251	OW0	HOH	X	80	27.963	46.174	57.087	1.00	7.67
12254	OW0	HOH	X	81	11.021	38.002	66.975	1.00	15.55
12257	OW0	HOH	X	82	51.837	43.690	68.342	1.00	10.61
12260	OW0	HOH	X	85	1.727	54.318	84.323	1.00	19.85
12263	OW0	HOH	X	86	22.017	55.208	87.937	1.00	16.95
12266	OW0	HOH	X	87	11.197	59.757	83.177	1.00	10.32
12269	OW0	HOH	X	88	26.701	44.673	59.173	1.00	13.23
12272	OW0	HOH	X	89	17.203	18.725	63.349	1.00	16.94
12275	OW0	HOH	X	91	17.234	27.909	51.270	1.00	11.35
12278	OW0	HOH	X	92	40.319	10.753	43.477	1.00	11.18
12281	OW0	HOH	X	93	24.671	46.144	37.034	1.00	14.85
12284	OW0	HOH	X	94	50.497	39.564	59.626	1.00	15.99
12287	OW0	HOH	X	95	28.485	11.280	44.890	1.00	13.03
12290	OW0	HOH	X	96	26.076	29.955	36.770	1.00	14.67
12293	OW0	HOH	X	97	48.833	42.005	54.263	1.00	18.09
12296	OW0	HOH	X	98	49.499	49.343	87.677	1.00	9.66
12299	OW0	HOH	X	99	49.711	46.937	45.448	1.00	11.20
12302	OW0	HOH	X	100	17.034	30.213	63.021	1.00	15.07
12305	OW0	HOH	X	101	39.683	15.310	34.487	1.00	13.75
12308	OW0	HOH	X	102	44.335	11.635	41.805	1.00	13.31
12311	OW0	HOH	X	103	7.317	27.909	36.212	1.00	11.34
12314	OW0	HOH	X	104	14.704	56.815	66.265	1.00	8.90
12317	OW0	HOH	X	105	30.994	21.544	31.303	1.00	12.47
12320	OW0	HOH	X	106	19.105	28.070	43.772	1.00	10.04
12323	OW0	HOH	X	107	16.387	23.911	71.997	1.00	11.90
12326	OW0	HOH	X	108	48.313	16.191	38.471	1.00	12.69
12329	OW0	HOH	X	109	25.622	39.494	84.415	1.00	24.88
12332	OW0	HOH	X	110	50.581	54.685	69.555	1.00	8.32
12335	OW0	HOH	X	112	53.769	12.589	45.674	1.00	18.44
12338	OW0	HOH	X	113	7.739	47.306	69.980	1.00	10.75
12341	OW0	HOH	X	118	24.718	48.774	36.583	1.00	34.55
12344	OW0	HOH	X	119	7.420	57.013	83.641	1.00	8.77
12347	OW0	HOH	X	120	19.006	22.639	65.181	1.00	10.40
12350	OW0	HOH	X	121	22.850	31.469	59.584	1.00	9.47
12353	OW0	HOH	X	123	27.592	19.750	72.231	1.00	11.90
12356	OW0	HOH	X	125	29.354	39.792	76.111	1.00	8.32
12359	OW0	HOH	X	126	16.312	16.791	46.836	1.00	10.25
12362	OW0	HOH	X	127	36.004	9.585	45.288	1.00	9.94
12365	OW0	HOH	X	128	46.313	19.045	63.863	1.00	11.02
12368	OW0	HOH	X	129	18.034	51.502	71.454	1.00	9.13
12371	OW0	HOH	X	130	20.505	42.254	61.270	1.00	11.65
12374	OW0	HOH	X	131	22.608	62.182	68.933	1.00	15.02

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
12377	OW0	HOH	X	134	14.312	64.302	77.403	1.00	7.67
12380	OW0	HOH	X	135	11.028	39.535	74.451	1.00	19.43
12383	OW0	HOH	X	136	14.223	26.650	27.585	1.00	12.87
12386	OW0	HOH	X	137	43.057	31.784	65.159	1.00	11.35
12389	OW0	HOH	X	138	58.106	28.609	35.191	1.00	14.89
12392	OW0	HOH	X	139	23.212	58.740	83.180	1.00	10.87
12395	OW0	HOH	X	140	38.561	27.948	95.698	1.00	10.41
12398	OW0	HOH	X	141	45.194	30.542	83.718	1.00	14.50
12401	OW0	HOH	X	142	41.728	58.102	67.430	1.00	10.85
12404	OW0	HOH	X	144	37.008	49.713	42.286	1.00	12.61
12407	OW0	HOH	X	145	26.901	50.339	36.521	1.00	7.56
12410	OW0	HOH	X	146	50.276	48.399	70.764	1.00	18.66
12413	OW0	HOH	X	147	53.455	26.850	27.856	1.00	16.15
12416	OW0	HOH	X	148	18.143	14.600	34.283	1.00	22.79
12419	OW0	HOH	X	150	23.128	44.982	82.122	1.00	18.72
12422	OW0	HOH	X	151	16.326	28.490	43.994	1.00	8.79
12425	OW0	HOH	X	152	19.740	48.939	82.310	1.00	9.93
12428	OW0	HOH	X	153	4.832	45.171	81.797	1.00	20.26
12431	OW0	HOH	X	154	44.638	59.170	64.359	1.00	18.50
12434	OW0	HOH	X	156	16.284	41.917	46.650	1.00	12.36
12437	OW0	HOH	X	157	27.192	60.806	76.452	1.00	13.73
12440	OW0	HOH	X	158	30.835	6.332	40.927	1.00	16.00
12443	OW0	HOH	X	159	21.876	51.233	92.307	1.00	23.93
12446	OW0	HOH	X	160	43.013	51.452	76.998	1.00	8.07
12449	OW0	HOH	X	161	18.775	36.954	33.092	1.00	14.54
12452	OW0	HOH	X	162	15.236	31.821	59.143	1.00	12.63
12455	OW0	HOH	X	164	18.617	51.118	66.094	1.00	10.12
12458	OW0	HOH	X	166	49.374	13.222	51.347	1.00	9.60
12461	OW0	HOH	X	167	49.931	36.538	77.121	1.00	10.30
12464	OW0	HOH	X	168	2.809	51.944	87.715	1.00	15.56
12467	OW0	HOH	X	169	53.597	61.143	61.047	1.00	15.24
12470	OW0	HOH	X	171	44.069	33.976	64.052	1.00	10.69
12473	OW0	HOH	X	172	52.540	24.738	56.320	1.00	12.53
12476	OW0	HOH	X	173	39.216	31.924	103.001	1.00	22.82
12479	OW0	HOH	X	174	19.667	24.480	78.285	1.00	16.66
12482	O	HOH	X	175	24.755	54.772	46.478	1.00	14.47
12485	O	HOH	X	176	24.979	52.683	44.876	1.00	11.41
12488	O	HOH	X	177	27.462	51.379	44.522	1.00	12.37
12491	O	HOH	X	178	29.011	53.276	45.703	1.00	22.84
12494	O	HOH	X	179	26.403	56.744	48.957	1.00	20.79
12497	O	HOH	X	180	35.465	61.181	42.400	1.00	13.93
12500	O	HOH	X	181	35.452	58.415	42.353	1.00	20.51
12503	O	HOH	X	182	32.776	57.084	42.854	1.00	24.59
12506	O	HOH	X	183	31.113	63.894	43.390	1.00	20.49
12509	O	HOH	X	184	32.114	65.989	45.232	1.00	23.59
12512	O	HOH	X	185	33.229	70.197	44.488	1.00	11.83
12515	O	HOH	X	186	26.349	69.956	44.469	1.00	12.36
12518	O	HOH	X	187	25.968	69.575	47.056	1.00	22.01
12521	O	HOH	X	188	30.000	70.650	47.360	1.00	19.57
12524	O	HOH	X	189	24.858	64.738	46.936	1.00	20.71
12527	O	HOH	X	190	24.236	37.355	49.741	1.00	17.95
12530	O	HOH	X	191	22.865	34.718	49.470	1.00	17.44

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
12533	O	HOH	X	192	55.875	37.887	52.950	1.00	24.93
12536	O	HOH	X	193	55.055	31.546	49.094	1.00	17.24
12539	O	HOH	X	194	56.005	29.887	46.941	1.00	19.43
12542	O	HOH	X	195	56.288	28.168	31.339	1.00	17.94
12545	O	HOH	X	196	57.575	35.180	31.963	1.00	11.21
12548	O	HOH	X	197	59.355	31.084	29.185	1.00	17.13
12551	O	HOH	X	198	57.931	32.043	25.167	1.00	12.98
12554	O	HOH	X	199	58.125	34.690	24.527	1.00	24.77
12557	O	HOH	X	200	56.681	34.627	21.202	1.00	13.50
12560	O	HOH	X	201	17.778	44.310	43.692	1.00	20.65
12563	O	HOH	X	202	16.269	40.538	41.405	1.00	17.69
12566	O	HOH	X	203	13.079	36.714	40.768	1.00	13.52
12569	O	HOH	X	204	17.634	32.074	86.662	1.00	17.50
12572	O	HOH	X	205	11.621	26.838	74.001	1.00	27.56
12575	O	HOH	X	206	13.067	27.428	71.840	1.00	11.46
12578	O	HOH	X	207	10.848	27.375	70.113	1.00	21.23
12581	O	HOH	X	208	5.740	43.597	89.229	1.00	22.03
12584	O	HOH	X	209	39.732	28.662	42.301	1.00	29.18
12587	O	HOH	X	210	19.393	46.253	59.822	1.00	21.96
12590	O	HOH	X	211	18.101	47.600	55.300	1.00	17.10
12593	O	HOH	X	212	16.143	49.623	58.989	1.00	21.68
12596	O	HOH	X	213	7.455	38.767	75.293	1.00	23.21
12599	O	HOH	X	214	9.895	37.361	75.847	1.00	20.38
12602	O	HOH	X	215	11.175	37.040	78.126	1.00	14.50
12605	O	HOH	X	216	9.007	38.082	68.602	1.00	21.88
12608	O	HOH	X	217	11.732	39.968	71.693	1.00	10.91
12611	O	HOH	X	218	9.728	33.470	77.480	1.00	13.86
12614	O	HOH	X	219	10.037	28.690	79.135	1.00	17.57
12617	O	HOH	X	220	20.339	40.116	67.297	1.00	17.59
12620	O	HOH	X	221	20.091	43.126	67.388	1.00	18.87
12623	O	HOH	X	222	27.995	36.212	40.563	1.00	8.23
12626	O	HOH	X	223	5.037	18.451	53.748	1.00	20.55
12629	O	HOH	X	224	7.871	14.917	54.622	1.00	21.87
12632	O	HOH	X	225	6.090	13.077	53.204	1.00	18.43
12635	O	HOH	X	226	6.842	11.579	51.072	1.00	19.50
12638	O	HOH	X	227	6.694	20.091	61.060	1.00	25.26
12641	O	HOH	X	228	6.116	22.445	62.342	1.00	15.47
12644	O	HOH	X	229	3.431	22.218	61.416	1.00	23.60
12647	O	HOH	X	230	2.936	21.420	56.473	1.00	13.56
12650	O	HOH	X	231	1.345	23.314	62.597	1.00	21.70
12653	O	HOH	X	232	20.854	12.085	50.599	1.00	16.66
12656	O	HOH	X	233	22.967	14.270	46.618	1.00	20.55
12659	O	HOH	X	234	20.297	13.469	45.850	1.00	15.82
12662	O	HOH	X	235	17.819	14.121	46.590	1.00	25.66
12665	O	HOH	X	236	24.675	12.693	48.148	1.00	32.57
12668	O	HOH	X	237	23.905	12.556	44.212	1.00	21.44
12671	O	HOH	X	238	25.984	10.843	43.868	1.00	18.00
12674	O	HOH	X	239	21.872	10.445	43.853	1.00	31.66
12677	O	HOH	X	240	42.344	10.274	45.421	1.00	20.25
12680	O	HOH	X	241	38.163	8.970	43.542	1.00	16.98
12683	O	HOH	X	242	7.689	45.214	81.716	1.00	11.77
12686	O	HOH	X	243	8.997	43.305	83.201	1.00	15.34

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
12689	O	HOH	X	244	17.118	54.258	88.389	1.00	27.91
12692	O	HOH	X	245	15.185	56.757	89.749	1.00	36.24
12695	O	HOH	X	246	29.876	11.951	67.175	1.00	21.22
12698	O	HOH	X	247	27.277	11.882	61.263	1.00	35.35
12701	O	HOH	X	248	31.389	11.807	58.176	1.00	20.07
12704	O	HOH	X	249	37.938	10.860	55.565	1.00	22.84
12707	O	HOH	X	250	34.793	10.010	56.141	1.00	25.66
12710	O	HOH	X	251	24.825	10.789	52.260	1.00	31.45
12713	O	HOH	X	252	28.151	13.670	51.691	1.00	18.08
12716	O	HOH	X	253	29.430	13.503	48.812	1.00	24.06
12719	O	HOH	X	254	12.748	32.216	53.697	1.00	25.41
12722	O	HOH	X	255	14.006	30.573	51.911	1.00	31.83
12725	O	HOH	X	256	14.884	28.000	52.679	1.00	20.24
12728	O	HOH	X	257	15.339	27.778	47.143	1.00	14.28
12731	O	HOH	X	258	15.571	31.486	48.111	1.00	21.83
12734	O	HOH	X	259	13.483	24.227	29.165	1.00	16.64
12737	O	HOH	X	260	37.334	41.126	28.388	1.00	32.43
12740	O	HOH	X	261	41.224	41.496	31.259	1.00	16.82
12743	O	HOH	X	262	55.320	44.552	42.643	1.00	15.92
12746	O	HOH	X	263	53.948	43.823	39.700	1.00	19.01
12749	O	HOH	X	264	52.132	47.502	46.431	1.00	16.47
12752	O	HOH	X	265	53.920	48.726	49.602	1.00	23.81
12755	O	HOH	X	266	55.907	46.381	51.001	1.00	23.25
12758	O	HOH	X	267	47.976	46.511	37.562	1.00	28.41
12761	O	HOH	X	268	37.795	23.464	74.898	1.00	18.96
12764	O	HOH	X	269	40.481	22.726	72.967	1.00	25.27
12767	O	HOH	X	270	51.470	17.307	70.892	1.00	30.35
12770	O	HOH	X	271	39.737	15.262	50.259	1.00	18.58
12773	O	HOH	X	272	43.912	15.519	59.886	1.00	24.46
12776	O	HOH	X	273	46.651	16.342	63.985	1.00	21.78
12779	O	HOH	X	274	45.106	15.419	66.003	1.00	23.01
12782	O	HOH	X	275	41.888	14.117	69.558	1.00	24.05
12785	O	HOH	X	276	40.912	12.292	67.638	1.00	17.83
12788	O	HOH	X	277	33.822	11.006	67.513	1.00	18.51
12791	O	HOH	X	278	50.556	12.442	45.084	1.00	13.89
12794	O	HOH	X	279	49.512	8.691	50.082	1.00	27.01
12797	O	HOH	X	280	49.349	10.516	52.038	1.00	23.77
12800	O	HOH	X	281	46.879	8.584	55.188	1.00	21.84
12803	O	HOH	X	282	35.899	42.525	32.875	1.00	19.60
12806	O	HOH	X	283	31.401	41.362	32.155	1.00	18.32
12809	O	HOH	X	284	23.611	38.853	32.115	1.00	17.00
12812	O	HOH	X	285	22.116	37.635	30.066	1.00	21.60
12815	O	HOH	X	286	19.630	36.740	30.533	1.00	17.38
12818	O	HOH	X	287	17.733	38.081	29.111	1.00	24.87
12821	O	HOH	X	288	15.158	38.582	30.365	1.00	21.75
12824	O	HOH	X	289	21.952	39.174	28.007	1.00	31.47
12827	O	HOH	X	290	21.847	39.259	25.176	1.00	24.78
12830	O	HOH	X	291	22.590	37.714	22.899	1.00	21.69
12833	O	HOH	X	292	18.700	31.297	22.487	1.00	19.45
12836	O	HOH	X	293	14.691	28.374	21.492	1.00	37.20
12839	O	HOH	X	294	19.811	26.767	21.127	1.00	29.13
12842	O	HOH	X	295	19.461	40.228	18.306	1.00	15.58

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
12845	O	HOH	X	296	53.757	46.767	62.397	1.00	24.50
12848	O	HOH	X	297	53.847	49.252	61.562	1.00	27.75
12851	O	HOH	X	298	53.025	51.368	63.486	1.00	12.86
12854	O	HOH	X	299	54.081	52.743	69.926	1.00	15.78
12857	O	HOH	X	300	55.971	50.155	72.085	1.00	30.97
12860	O	HOH	X	301	57.259	53.959	68.699	1.00	29.61
12863	O	HOH	X	302	45.259	56.746	59.234	1.00	18.17
12866	O	HOH	X	303	48.099	55.948	60.118	1.00	20.59
12869	O	HOH	X	304	28.107	17.450	68.352	1.00	13.92
12872	O	HOH	X	305	21.426	15.480	67.000	1.00	24.46
12875	O	HOH	X	306	24.704	19.923	70.054	1.00	22.84
12878	O	HOH	X	307	16.803	22.717	74.616	1.00	25.93
12881	O	HOH	X	308	18.460	22.664	76.692	1.00	20.75
12884	O	HOH	X	309	26.027	21.825	68.652	1.00	13.28
12887	O	HOH	X	310	31.822	20.284	82.401	1.00	15.61
12890	O	HOH	X	311	34.019	18.610	82.738	1.00	18.36
12893	O	HOH	X	312	39.344	17.074	80.869	1.00	20.70
12896	O	HOH	X	313	27.432	25.734	94.654	1.00	31.09
12899	O	HOH	X	314	26.414	27.986	87.227	1.00	22.40
12902	O	HOH	X	315	24.954	25.448	88.249	1.00	24.87
12905	O	HOH	X	316	24.325	23.866	86.217	1.00	30.14
12908	O	HOH	X	317	29.587	22.071	91.620	1.00	33.57
12911	O	HOH	X	318	30.980	24.379	92.105	1.00	29.46
12914	O	HOH	X	319	14.731	35.754	85.338	1.00	23.23
12917	O	HOH	X	320	12.364	33.893	84.405	1.00	31.62
12920	O	HOH	X	321	14.417	31.878	84.905	1.00	25.48
12923	O	HOH	X	322	23.284	41.523	94.438	1.00	25.80
12926	O	HOH	X	323	29.007	42.318	97.631	1.00	17.04
12929	O	HOH	X	324	27.723	40.249	94.113	1.00	21.17
12932	O	HOH	X	325	26.887	41.076	96.388	1.00	25.45
12935	O	HOH	X	326	28.438	39.009	99.971	1.00	22.94
12938	O	HOH	X	327	30.486	40.540	99.099	1.00	19.65
12941	O	HOH	X	328	28.496	48.427	94.049	1.00	21.62
12944	O	HOH	X	329	27.553	47.561	91.585	1.00	23.53
12947	O	HOH	X	330	32.296	54.435	89.240	1.00	18.76
12950	O	HOH	X	331	29.701	55.028	90.167	1.00	14.15
12953	O	HOH	X	332	27.507	54.570	88.708	1.00	18.39
12956	O	HOH	X	333	26.192	52.157	88.738	1.00	12.85
12959	O	HOH	X	334	31.773	51.995	92.467	1.00	24.07
12962	O	HOH	X	335	33.640	56.155	91.898	1.00	35.79
12965	O	HOH	X	336	29.383	53.094	92.184	1.00	31.80
12968	O	HOH	X	337	41.297	46.407	101.493	1.00	16.85
12971	O	HOH	X	338	39.054	47.121	99.839	1.00	25.81
12974	O	HOH	X	339	43.154	48.533	101.599	1.00	19.90
12977	O	HOH	X	340	5.500	58.089	72.276	1.00	8.90
12980	O	HOH	X	341	6.875	63.597	74.790	1.00	12.03
12983	O	HOH	X	342	4.929	65.692	72.097	1.00	38.25
12986	O	HOH	X	343	5.626	60.056	67.977	1.00	15.05
12989	O	HOH	X	344	8.303	56.605	66.193	1.00	16.70
12992	O	HOH	X	345	-2.884	57.735	80.711	1.00	16.41
12995	O	HOH	X	346	-4.177	55.723	81.677	1.00	13.40
12998	O	HOH	X	347	-5.925	58.170	77.409	1.00	17.94

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
13001	O	HOH	X	348	-10.014	55.560	79.627	1.00	19.31
13004	O	HOH	X	349	7.762	58.248	85.951	1.00	21.03
13007	O	HOH	X	350	6.209	61.419	85.241	1.00	16.16
13010	O	HOH	X	351	5.408	59.664	87.032	1.00	30.08
13013	O	HOH	X	352	13.192	50.137	88.827	1.00	27.97
13016	O	HOH	X	353	19.027	40.519	77.372	1.00	8.11
13019	O	HOH	X	354	49.087	30.538	52.830	1.00	17.93
13022	O	HOH	X	355	47.478	31.069	54.724	1.00	35.94
13025	O	HOH	X	356	49.981	30.266	60.977	1.00	24.32
13028	O	HOH	X	357	55.493	19.161	49.511	1.00	17.79
13031	O	HOH	X	358	55.388	17.015	51.125	1.00	19.34
13034	O	HOH	X	359	53.941	22.671	61.547	1.00	20.83
13037	O	HOH	X	360	51.986	21.902	63.319	1.00	25.50
13040	O	HOH	X	361	52.901	24.443	65.252	1.00	23.10
13043	O	HOH	X	362	47.408	20.768	70.780	1.00	24.47
13046	O	HOH	X	363	45.542	22.482	73.294	1.00	31.27
13049	O	HOH	X	364	42.981	25.939	75.651	1.00	27.14
13052	O	HOH	X	365	47.297	40.701	94.829	1.00	20.58
13055	O	HOH	X	366	43.675	31.763	88.313	1.00	20.66
13058	O	HOH	X	367	45.418	35.010	91.974	1.00	20.60
13061	O	HOH	X	368	46.497	27.385	93.574	1.00	14.46
13064	O	HOH	X	369	48.922	28.965	94.260	1.00	20.08
13067	O	HOH	X	370	45.913	31.040	94.657	1.00	28.35
13070	O	HOH	X	371	22.247	45.971	38.845	1.00	23.72
13073	O	HOH	X	372	21.204	45.452	41.489	1.00	19.50
13076	O	HOH	X	373	27.207	48.158	55.433	1.00	21.48
13079	O	HOH	X	374	24.882	48.062	53.589	1.00	17.59
13082	O	HOH	X	375	25.252	50.715	53.634	1.00	11.81
13085	O	HOH	X	376	19.961	61.130	50.349	1.00	20.01
13088	O	HOH	X	377	10.761	65.286	59.048	1.00	40.59
13091	O	HOH	X	378	17.961	62.676	49.988	1.00	25.56
13094	O	HOH	X	379	15.342	63.547	53.248	1.00	18.81
13097	O	HOH	X	380	14.325	66.690	50.023	1.00	21.09
13100	O	HOH	X	381	14.499	69.131	51.220	1.00	37.41
13103	O	HOH	X	382	20.362	58.939	45.873	1.00	26.90
13106	O	HOH	X	383	19.800	61.904	45.998	1.00	31.62
13109	O	HOH	X	384	17.880	65.600	57.263	1.00	18.70
13112	O	HOH	X	385	16.728	64.337	39.667	1.00	13.00
13115	O	HOH	X	386	16.223	59.605	45.082	1.00	25.78
13118	O	HOH	X	387	14.189	56.822	46.793	1.00	23.52
13121	O	HOH	X	388	13.594	59.907	48.301	1.00	27.64
13124	O	HOH	X	389	16.763	53.016	46.768	1.00	22.02
13127	O	HOH	X	390	17.665	54.085	49.162	1.00	14.60
13130	O	HOH	X	391	19.053	55.899	44.598	1.00	20.55
13133	O	HOH	X	392	43.866	23.316	30.312	1.00	21.04
13136	O	HOH	X	393	41.373	21.824	31.171	1.00	24.00
13139	O	HOH	X	394	40.976	19.564	32.272	1.00	25.58
13142	O	HOH	X	395	39.255	22.629	30.002	1.00	26.43
13145	O	HOH	X	396	43.971	18.647	32.602	1.00	30.42
13148	O	HOH	X	397	35.939	16.411	35.220	1.00	14.57
13151	O	HOH	X	398	25.361	17.252	35.431	1.00	9.94
13154	O	HOH	X	399	26.768	18.578	74.723	1.00	20.37

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
13157	O	HOH	X	400	37.081	28.754	99.468	1.00	18.08
13160	O	HOH	X	401	39.299	30.235	100.333	1.00	33.34
13163	O	HOH	X	402	38.086	34.906	94.487	1.00	35.56
13166	O	HOH	X	403	34.173	38.259	90.722	1.00	13.01
13169	O	HOH	X	404	30.792	40.748	85.282	1.00	13.76
13172	O	HOH	X	405	48.556	33.288	75.704	1.00	27.62
13175	O	HOH	X	406	47.764	32.794	71.259	1.00	18.90
13178	O	HOH	X	407	53.326	31.949	70.529	1.00	30.45
13181	O	HOH	X	408	35.510	32.479	51.024	1.00	7.19
13184	O	HOH	X	409	36.943	34.247	47.574	1.00	8.51
13187	O	HOH	X	410	35.377	32.126	46.876	1.00	5.55
13190	O	HOH	X	411	29.437	42.669	49.946	1.00	6.94
13193	O	HOH	X	412	26.463	39.530	62.409	1.00	8.61
13196	O	HOH	X	413	23.875	40.113	62.595	1.00	8.81
13199	O	HOH	X	414	23.355	38.555	59.001	1.00	7.41
13202	O	HOH	X	415	20.633	36.302	55.089	1.00	11.50
13205	O	HOH	X	416	24.583	36.286	55.828	1.00	11.52
13208	O	HOH	X	417	26.706	35.543	57.299	1.00	8.12
13211	O	HOH	X	418	18.333	37.785	54.184	1.00	20.35
13214	O	HOH	X	419	20.772	29.575	53.661	1.00	10.11
13217	O	HOH	X	420	18.315	29.949	52.639	1.00	17.01
13220	O	HOH	X	421	17.202	28.889	48.827	1.00	10.77
13223	O	HOH	X	422	24.798	57.374	51.059	1.00	10.20
13226	O	HOH	X	423	8.702	42.173	70.339	1.00	24.94
13229	O	HOH	X	424	7.253	44.942	69.014	1.00	19.53
13232	O	HOH	X	425	8.227	49.360	68.337	1.00	18.47
13235	O	HOH	X	426	12.217	49.061	66.748	1.00	19.81
13238	O	HOH	X	427	16.551	44.873	64.042	1.00	20.15
13241	O	HOH	X	428	15.817	49.587	65.433	1.00	19.52
13244	O	HOH	X	429	18.410	46.149	67.202	1.00	26.92
13247	O	HOH	X	430	20.146	51.767	64.197	1.00	25.26
13250	O	HOH	X	431	19.359	52.508	61.742	1.00	24.78
13253	O	HOH	X	432	15.030	60.723	57.139	1.00	19.57
13256	O	HOH	X	433	4.817	50.769	89.133	1.00	15.28
13259	O	HOH	X	434	11.907	22.681	64.300	1.00	13.09
13262	O	HOH	X	435	12.032	23.024	67.077	1.00	19.39
13265	O	HOH	X	436	10.050	21.369	67.429	1.00	23.70
13268	O	HOH	X	437	12.750	18.583	65.522	1.00	25.02
13271	O	HOH	X	438	14.617	22.209	67.576	1.00	21.11
13274	O	HOH	X	439	16.121	21.911	65.430	1.00	14.75
13277	O	HOH	X	440	16.013	19.249	65.564	1.00	25.78
13280	O	HOH	X	441	12.826	15.595	61.077	1.00	18.47
13283	O	HOH	X	442	13.850	19.610	68.358	1.00	29.96
13286	O	HOH	X	443	45.065	30.009	71.586	1.00	23.21
13289	O	HOH	X	444	49.416	27.426	72.720	1.00	24.73
13292	O	HOH	X	445	51.651	40.791	85.344	1.00	20.44
13295	O	HOH	X	446	56.174	37.189	77.532	1.00	33.26
13298	O	HOH	X	447	53.393	42.572	83.764	1.00	15.79
13301	O	HOH	X	448	50.894	48.723	81.385	1.00	8.20
13304	O	HOH	X	449	52.163	51.286	81.016	1.00	25.40
13307	O	HOH	X	450	54.393	46.882	81.953	1.00	31.73
13310	O	HOH	X	451	53.693	46.898	77.730	1.00	29.70

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
13313	O	HOH	X	452	21.627	41.245	39.048	1.00	16.54
13316	O	HOH	X	453	16.987	40.328	58.483	1.00	24.90
13319	O	HOH	X	454	22.149	43.484	37.745	1.00	23.19
13322	O	HOH	X	455	19.349	43.366	36.713	1.00	29.42
13325	O	HOH	X	456	21.851	44.904	33.285	1.00	32.85
13328	O	HOH	X	457	14.763	39.091	52.663	1.00	23.00
13331	O	HOH	X	458	12.565	41.532	55.794	1.00	24.86
13334	O	HOH	X	459	14.587	42.736	57.649	1.00	22.57
13337	O	HOH	X	460	14.635	49.015	55.320	1.00	25.40
13340	O	HOH	X	461	17.743	42.308	60.772	1.00	23.60
13343	O	HOH	X	462	14.136	39.330	55.219	1.00	27.56
13346	O	HOH	X	463	13.610	36.778	55.422	1.00	38.60
13349	O	HOH	X	464	13.241	34.166	55.656	1.00	30.81
13352	O	HOH	X	465	13.653	33.641	58.222	1.00	24.59
13355	O	HOH	X	466	11.052	36.056	59.115	1.00	24.92
13358	O	HOH	X	467	8.638	39.731	61.330	1.00	30.60
13361	O	HOH	X	468	13.708	29.666	60.039	1.00	22.42
13364	O	HOH	X	469	18.344	37.662	91.022	1.00	28.31
13367	O	HOH	X	470	17.627	37.703	88.360	1.00	23.87
13370	O	HOH	X	471	22.581	43.114	90.894	1.00	20.24
13373	O	HOH	X	472	21.787	30.931	91.396	1.00	18.65
13376	O	HOH	X	473	18.713	28.872	92.977	1.00	32.82
13379	O	HOH	X	474	22.273	29.414	93.999	1.00	27.75
13382	O	HOH	X	475	26.002	30.630	96.979	1.00	24.07
13385	O	HOH	X	476	27.258	32.757	98.114	1.00	28.08
13388	O	HOH	X	477	30.014	44.816	97.444	1.00	16.92
13391	O	HOH	X	478	15.911	52.518	70.059	1.00	11.43
13394	O	HOH	X	479	18.244	50.023	73.495	1.00	12.08
13397	O	HOH	X	480	46.942	39.940	28.387	1.00	27.79
13400	O	HOH	X	481	49.601	42.760	32.126	1.00	21.03
13403	O	HOH	X	482	41.317	47.091	35.248	1.00	29.34
13406	O	HOH	X	483	35.975	51.978	43.568	1.00	22.00
13409	O	HOH	X	484	31.504	52.682	46.494	1.00	14.97
13412	O	HOH	X	485	26.979	26.083	75.207	1.00	30.74
13415	O	HOH	X	486	46.763	35.441	60.103	1.00	17.85
13418	O	HOH	X	487	51.024	35.379	57.107	1.00	29.28
13421	O	HOH	X	488	57.413	33.980	49.905	1.00	30.63
13424	O	HOH	X	489	57.424	35.520	36.073	1.00	12.13
13427	O	HOH	X	490	60.248	35.561	36.195	1.00	25.63
13430	O	HOH	X	491	57.804	39.324	35.239	1.00	24.61
13433	O	HOH	X	492	53.358	36.717	23.959	1.00	25.99
13436	O	HOH	X	493	55.320	37.740	25.527	1.00	21.74
13439	O	HOH	X	494	46.690	35.384	25.641	1.00	26.54
13442	O	HOH	X	495	47.631	26.123	25.356	1.00	18.30
13445	O	HOH	X	496	47.036	28.020	27.265	1.00	14.94
13448	O	HOH	X	497	44.452	27.382	27.723	1.00	22.88
13451	O	HOH	X	498	22.675	64.741	56.316	1.00	14.76
13454	O	HOH	X	499	20.302	66.617	57.360	1.00	31.53
13457	O	HOH	X	500	19.055	66.083	72.327	1.00	25.86
13460	O	HOH	X	501	16.790	64.632	73.423	1.00	28.26
13463	O	HOH	X	502	15.743	63.356	71.407	1.00	27.95
13466	O	HOH	X	503	20.680	70.403	71.730	1.00	47.23

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FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
13469	O	HOH	X	504	16.988	75.350	58.359	1.00	24.53
13472	O	HOH	X	505	17.567	71.729	61.679	1.00	13.72
13475	O	HOH	X	506	19.567	73.569	60.956	1.00	27.61
13478	O	HOH	X	507	20.314	76.024	61.801	1.00	36.01
13481	O	HOH	X	508	18.825	77.930	62.565	1.00	24.53
13484	O	HOH	X	509	6.533	41.760	90.903	1.00	29.00
13487	O	HOH	X	510	26.070	41.219	25.871	1.00	36.27
13490	O	HOH	X	511	10.045	41.256	81.814	1.00	24.00
13493	O	HOH	X	512	7.317	40.616	81.247	1.00	23.74
13496	O	HOH	X	513	6.931	42.438	84.787	1.00	25.43
13499	O	HOH	X	514	5.196	42.322	86.856	1.00	24.68
13502	O	HOH	X	515	3.579	45.863	79.410	1.00	26.22
13505	O	HOH	X	516	2.949	49.709	79.123	1.00	19.81
13508	O	HOH	X	517	3.787	50.983	75.264	1.00	20.59
13511	O	HOH	X	518	3.543	47.726	72.803	1.00	23.74
13514	O	HOH	X	519	15.301	29.140	84.208	1.00	18.79
13517	O	HOH	X	520	17.711	29.466	85.365	1.00	27.73
13520	O	HOH	X	521	18.184	31.284	89.201	1.00	32.32
13523	O	HOH	X	522	22.534	25.366	89.272	1.00	26.37
13526	O	HOH	X	523	20.096	33.514	92.954	1.00	29.11
13529	O	HOH	X	524	20.910	37.959	94.854	1.00	25.95
13532	O	HOH	X	525	20.631	36.346	92.769	1.00	26.92
13535	O	HOH	X	526	35.247	7.081	61.117	1.00	22.65
13538	O	HOH	X	527	32.414	9.481	60.755	1.00	30.25
13541	O	HOH	X	528	37.184	11.554	53.025	1.00	26.37
13544	O	HOH	X	529	41.789	11.189	52.874	1.00	20.67
13547	O	HOH	X	530	30.631	11.131	50.004	1.00	27.43
13550	O	HOH	X	531	33.049	10.802	50.629	1.00	30.29
13553	O	HOH	X	532	29.255	11.253	52.355	1.00	28.94
13556	O	HOH	X	533	29.100	8.815	45.737	1.00	24.92
13559	O	HOH	X	534	26.027	8.035	44.373	1.00	29.78
13562	O	HOH	X	535	30.897	7.578	43.939	1.00	29.33
13565	O	HOH	X	536	37.728	6.345	42.827	1.00	14.73
13568	O	HOH	X	537	41.632	8.110	46.570	1.00	33.75
13571	O	HOH	X	538	41.698	11.516	41.300	1.00	21.02
13574	O	HOH	X	539	44.336	14.941	38.940	1.00	16.97
13577	O	HOH	X	540	42.609	12.928	37.519	1.00	17.06
13580	O	HOH	X	541	47.827	19.539	33.922	1.00	18.67
13583	O	HOH	X	542	47.911	13.575	38.010	1.00	24.47
13586	O	HOH	X	543	45.906	13.098	40.136	1.00	22.40
13589	O	HOH	X	544	52.109	18.020	55.188	1.00	24.04
13592	O	HOH	X	545	55.179	25.152	55.761	1.00	24.94
13595	O	HOH	X	546	56.959	31.832	51.120	1.00	25.64
13598	O	HOH	X	547	56.362	29.809	54.608	1.00	33.37
13601	O	HOH	X	548	57.400	17.263	47.859	1.00	25.72
13604	O	HOH	X	549	57.831	14.739	47.458	1.00	31.24
13607	O	HOH	X	550	56.437	12.739	46.424	1.00	29.72
13610	O	HOH	X	551	54.403	18.534	53.681	1.00	27.18
13613	O	HOH	X	552	57.682	22.052	42.446	1.00	20.44
13616	O	HOH	X	553	58.658	24.548	43.826	1.00	31.62
13619	O	HOH	X	554	57.399	25.802	41.808	1.00	28.72
13622	O	HOH	X	555	54.007	21.789	37.840	1.00	24.27

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
13625	O	HOH	X	556	56.596	20.111	38.620	1.00	20.53
13628	O	HOH	X	557	57.632	23.143	39.131	1.00	25.41
13631	O	HOH	X	558	18.243	43.236	39.008	1.00	26.13
13634	O	HOH	X	559	24.641	43.230	36.310	1.00	25.39
13637	O	HOH	X	560	13.730	39.160	41.227	1.00	23.76
13640	O	HOH	X	561	20.298	40.795	41.981	1.00	21.27
13643	O	HOH	X	562	17.457	35.372	50.204	1.00	25.59
13646	O	HOH	X	563	20.274	33.501	48.130	1.00	25.82
13649	O	HOH	X	564	10.550	41.183	57.569	1.00	24.95
13652	O	HOH	X	565	12.027	42.780	53.580	1.00	25.57
13655	O	HOH	X	566	29.273	62.525	76.025	1.00	28.32
13658	O	HOH	X	567	31.523	62.817	77.548	1.00	23.35
13661	O	HOH	X	568	28.037	65.816	76.174	1.00	44.37
13664	O	HOH	X	569	26.024	67.463	73.989	1.00	32.45
13667	O	HOH	X	570	22.825	64.097	74.794	1.00	23.85
13670	O	HOH	X	571	33.726	60.717	77.777	1.00	19.54
13673	O	HOH	X	572	34.132	58.822	75.636	1.00	20.81
13676	O	HOH	X	573	32.823	59.240	73.388	1.00	24.12
13679	O	HOH	X	574	34.883	63.146	73.236	1.00	30.07
13682	O	HOH	X	575	37.087	59.423	72.313	1.00	15.26
13685	O	HOH	X	576	35.192	58.550	70.774	1.00	14.97
13688	O	HOH	X	577	38.578	62.134	71.345	1.00	32.41
13691	O	HOH	X	578	38.114	62.536	62.639	1.00	26.81
13694	O	HOH	X	579	32.528	59.391	56.055	1.00	20.50
13697	O	HOH	X	580	30.284	57.924	54.722	1.00	15.46
13700	O	HOH	X	581	28.987	55.664	52.074	1.00	22.70
13703	O	HOH	X	582	31.827	53.786	49.233	1.00	28.26
13706	O	HOH	X	583	33.242	56.818	51.215	1.00	30.26
13709	O	HOH	X	584	36.848	58.226	54.239	1.00	18.40
13712	O	HOH	X	585	38.920	57.075	52.962	1.00	24.63
13715	O	HOH	X	586	36.910	59.041	59.557	1.00	27.64
13718	O	HOH	X	587	41.852	50.848	51.930	1.00	15.74
13721	O	HOH	X	588	43.187	51.974	49.865	1.00	20.39
13724	O	HOH	X	589	39.459	49.063	43.187	1.00	21.99
13727	O	HOH	X	590	37.795	53.875	41.221	1.00	25.50
13730	O	HOH	X	591	36.851	51.385	40.128	1.00	19.60
13733	O	HOH	X	592	15.376	22.121	29.461	1.00	31.95
13736	O	HOH	X	593	14.159	19.849	30.357	1.00	25.96
13739	O	HOH	X	594	19.395	19.901	27.944	1.00	26.28
13742	O	HOH	X	595	18.615	15.389	31.606	1.00	29.09
13745	O	HOH	X	596	27.195	20.904	28.842	1.00	28.97
13748	O	HOH	X	597	28.706	20.088	31.297	1.00	18.65
13751	O	HOH	X	598	33.444	17.738	35.200	1.00	20.45
13754	O	HOH	X	599	35.543	22.055	31.006	1.00	22.18
13757	O	HOH	X	600	50.236	25.728	25.352	1.00	29.75
13760	O	HOH	X	601	51.165	25.730	28.109	1.00	28.95
13763	O	HOH	X	602	26.932	13.082	63.595	1.00	35.63
13766	O	HOH	X	603	25.128	15.308	67.695	1.00	24.94
13769	O	HOH	X	604	15.168	12.763	61.107	1.00	31.87
13772	O	HOH	X	605	23.198	8.108	55.420	1.00	32.28
13775	O	HOH	X	606	20.895	8.535	54.145	1.00	22.97
13778	O	HOH	X	607	21.333	9.475	51.696	1.00	31.53

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
13781	O	HOH	X	608	18.933	8.076	50.294	1.00	33.50
13784	O	HOH	X	609	18.584	16.462	63.163	1.00	17.32
13787	O	HOH	X	610	20.001	36.335	58.384	1.00	21.91
13790	O	HOH	X	611	20.036	28.642	62.602	1.00	17.90
13793	O	HOH	X	612	38.068	50.390	54.033	1.00	18.22
13796	O	HOH	X	613	35.406	55.414	46.895	1.00	33.60
13799	O	HOH	X	614	24.310	49.686	41.940	1.00	23.51
13802	O	HOH	X	615	44.933	12.419	59.663	1.00	28.60
13805	O	HOH	X	616	41.939	12.624	59.432	1.00	19.58
13808	O	HOH	X	617	43.476	12.033	63.268	1.00	32.73
13811	O	HOH	X	618	23.570	14.888	42.898	1.00	9.87
13814	O	HOH	X	619	27.745	12.466	47.203	1.00	29.35
13817	O	HOH	X	620	27.285	14.335	49.343	1.00	42.70
13820	O	HOH	X	621	26.162	13.002	53.175	1.00	25.31
13823	O	HOH	X	622	6.642	29.713	38.074	1.00	22.86
13826	O	HOH	X	623	6.951	28.764	42.710	1.00	20.71
13829	O	HOH	X	624	4.344	26.298	39.561	1.00	30.96
13832	O	HOH	X	625	5.574	23.617	40.784	1.00	24.72
13835	O	HOH	X	626	9.316	24.364	30.469	1.00	26.00
13838	O	HOH	X	627	8.556	21.508	32.474	1.00	22.36
13841	O	HOH	X	628	6.713	21.927	34.377	1.00	23.08
13844	O	HOH	X	629	6.989	23.579	36.560	1.00	27.01
13847	O	HOH	X	630	12.792	35.494	29.817	1.00	27.97
13850	O	HOH	X	631	10.838	34.619	33.520	1.00	21.30
13853	O	HOH	X	632	5.252	23.475	53.594	1.00	29.61
13856	O	HOH	X	633	7.509	20.576	50.768	1.00	21.42
13859	O	HOH	X	634	10.822	21.133	49.094	1.00	32.71
13862	O	HOH	X	635	9.217	14.371	56.897	1.00	18.50
13865	O	HOH	X	636	3.065	20.412	59.712	1.00	33.47
13868	O	HOH	X	637	1.195	19.586	62.191	1.00	25.83
13871	O	HOH	X	638	1.698	28.875	62.058	1.00	18.53
13874	O	HOH	X	639	4.594	27.854	67.016	1.00	19.97
13877	O	HOH	X	640	6.041	32.000	69.643	1.00	27.84
13880	O	HOH	X	641	4.971	30.281	64.365	1.00	22.85
13883	O	HOH	X	642	7.125	28.763	62.307	1.00	18.59
13886	O	HOH	X	643	7.927	34.300	70.775	1.00	29.37
13889	O	HOH	X	644	9.249	31.986	71.543	1.00	27.57
13892	O	HOH	X	645	8.546	25.258	69.680	1.00	27.16
13895	O	HOH	X	646	12.146	22.503	71.668	1.00	32.07
13898	O	HOH	X	647	9.146	34.991	74.540	1.00	27.62
13901	O	HOH	X	648	9.953	35.653	71.853	1.00	24.14
13904	O	HOH	X	649	9.609	38.252	71.188	1.00	30.75
13907	O	HOH	X	650	38.747	42.766	31.630	1.00	27.43
13910	O	HOH	X	651	38.261	30.763	30.474	1.00	21.93
13913	O	HOH	X	652	40.417	29.047	26.700	1.00	27.80
13916	O	HOH	X	653	33.205	37.721	30.596	1.00	19.64
13919	O	HOH	X	654	39.315	16.517	46.960	1.00	20.58
13922	O	HOH	X	655	31.094	15.403	48.156	1.00	26.65
13925	O	HOH	X	656	62.244	31.953	43.253	1.00	33.03
13928	O	HOH	X	657	55.933	30.432	44.302	1.00	27.59
13931	O	HOH	X	658	51.696	42.268	36.364	1.00	31.06
13934	O	HOH	X	659	54.520	40.328	37.482	1.00	23.46

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
13937	O	HOH	X	660	57.994	44.251	42.595	1.00	25.41
13940	O	HOH	X	661	49.544	47.984	42.942	1.00	23.39
13943	O	HOH	X	662	50.468	49.348	54.674	1.00	25.64
13946	O	HOH	X	663	50.136	51.103	52.859	1.00	29.50
13949	O	HOH	X	664	46.746	50.419	48.438	1.00	33.94
13952	O	HOH	X	665	54.059	47.230	66.336	1.00	27.46
13955	O	HOH	X	666	53.067	46.049	68.726	1.00	24.62
13958	O	HOH	X	667	52.319	46.733	71.415	1.00	32.92
13961	O	HOH	X	668	53.046	50.988	68.283	1.00	24.57
13964	O	HOH	X	669	52.702	50.769	71.661	1.00	32.67
13967	O	HOH	X	670	52.186	48.197	74.166	1.00	32.28
13970	O	HOH	X	671	40.276	61.922	82.481	1.00	28.96
13973	O	HOH	X	672	39.652	62.892	80.064	1.00	26.46
13976	O	HOH	X	673	36.438	63.075	79.978	1.00	24.55
13979	O	HOH	X	674	40.207	65.449	80.010	1.00	28.93
13982	O	HOH	X	675	37.672	61.328	75.799	1.00	26.02
13985	O	HOH	X	676	38.693	62.994	73.933	1.00	28.49
13988	O	HOH	X	678	39.320	51.075	80.234	1.00	30.67
13991	O	HOH	X	679	34.469	56.370	76.494	1.00	20.87
13994	O	HOH	X	680	41.562	52.320	79.258	1.00	15.43
13997	O	HOH	X	681	36.864	59.010	74.830	1.00	15.02
14000	O	HOH	X	682	53.562	50.436	74.303	1.00	34.55
14003	O	HOH	X	683	49.771	37.993	57.541	1.00	32.56
14006	O	HOH	X	684	50.355	40.291	55.802	1.00	24.54
14009	O	HOH	X	685	50.411	42.319	57.395	1.00	23.82
14012	O	HOH	X	686	61.136	24.224	40.064	1.00	33.36
14015	O	HOH	X	687	33.190	13.832	33.496	1.00	26.28
14018	O	HOH	X	688	5.961	30.693	46.914	1.00	31.94
14021	O	HOH	X	689	11.315	35.053	41.801	1.00	30.15
14024	O	HOH	X	690	8.236	31.564	38.823	1.00	25.45
14027	O	HOH	X	691	5.342	26.000	36.581	1.00	27.81
14030	O	HOH	X	692	7.539	22.499	38.947	1.00	28.57
14033	O	HOH	X	693	5.708	28.951	53.613	1.00	30.35
14036	O	HOH	X	694	3.538	35.162	57.952	1.00	27.69
14039	O	HOH	X	695	6.983	34.404	64.765	1.00	25.04
14042	O	HOH	X	696	44.250	28.266	74.329	1.00	27.75
14045	O	HOH	X	697	42.789	24.603	71.575	1.00	24.65
14048	O	HOH	X	698	42.238	24.769	80.149	1.00	26.59
14051	O	HOH	X	699	40.080	23.509	95.230	1.00	26.29
14054	O	HOH	X	700	36.752	24.588	96.325	1.00	30.75
14057	O	HOH	X	701	38.811	24.977	98.597	1.00	25.57
14060	O	HOH	X	702	35.139	25.477	101.545	1.00	27.69
14063	O	HOH	X	703	35.612	42.931	99.544	1.00	34.22
14066	O	HOH	X	704	34.532	40.965	100.992	1.00	28.88
14069	O	HOH	X	705	33.627	46.599	97.466	1.00	20.68
14072	O	HOH	X	706	31.060	47.669	94.106	1.00	21.86
14075	O	HOH	X	707	32.419	49.680	93.309	1.00	25.11
14078	O	HOH	X	708	35.153	49.751	94.813	1.00	22.18
14081	O	HOH	X	709	26.931	50.680	91.231	1.00	26.22
14084	O	HOH	X	710	24.281	41.785	91.987	1.00	28.84
14087	O	HOH	X	711	20.179	42.551	95.164	1.00	38.86
14090	O	HOH	X	712	20.460	45.310	92.860	1.00	26.19

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
14093	O	HOH	X	713	24.023	19.802	74.920	1.00	38.27
14096	O	HOH	X	714	17.796	22.177	69.106	1.00	25.34
14099	O	HOH	X	715	14.208	23.066	75.382	1.00	28.32
14102	O	HOH	X	716	47.210	53.297	75.938	1.00	15.17
14105	O	HOH	X	717	56.258	36.855	61.432	1.00	28.50
14108	O	HOH	X	718	56.576	34.814	66.232	1.00	28.42
14111	O	HOH	X	719	54.879	35.855	69.799	1.00	21.85
14114	O	HOH	X	720	56.413	23.670	58.012	1.00	27.55
14117	O	HOH	X	721	57.014	21.427	58.803	1.00	25.17
14120	O	HOH	X	722	54.156	24.860	60.547	1.00	28.00
14123	O	HOH	X	723	48.569	15.495	65.677	1.00	26.17
14126	O	HOH	X	724	46.492	15.892	60.886	1.00	26.08
14129	O	HOH	X	725	29.775	27.682	49.207	1.00	18.56
14132	O	HOH	X	726	20.983	28.860	42.426	1.00	22.49
14135	O	HOH	X	727	17.069	17.850	67.700	1.00	31.25
14138	O	HOH	X	728	18.500	19.887	68.571	1.00	28.04
14141	O	HOH	X	729	28.606	11.264	64.668	1.00	26.44
14144	O	HOH	X	730	32.650	13.611	68.868	1.00	28.32
14147	O	HOH	X	731	39.538	18.167	71.076	1.00	24.46
14150	O	HOH	X	732	44.301	17.465	71.869	1.00	27.20
14153	O	HOH	X	733	35.443	16.334	74.420	1.00	23.20
14156	O	HOH	X	734	13.153	15.522	46.958	1.00	20.02
14159	O	HOH	X	735	12.470	19.150	45.655	1.00	30.24
14162	O	HOH	X	736	10.966	21.917	44.866	1.00	24.07
14165	O	HOH	X	737	33.369	54.110	40.895	1.00	34.94
14168	O	HOH	X	738	31.455	54.135	42.718	1.00	39.58
14171	O	HOH	X	739	47.576	49.203	46.362	1.00	23.31
14174	O	HOH	X	740	51.726	50.187	47.580	1.00	27.66
14177	O	HOH	X	741	52.870	46.396	53.036	1.00	26.52
14180	O	HOH	X	742	58.284	44.707	51.125	1.00	28.41
14183	O	HOH	X	743	57.821	51.105	49.694	1.00	29.49
14186	O	HOH	X	744	42.311	33.784	75.196	1.00	22.66
14189	O	HOH	X	745	43.030	33.840	77.638	1.00	20.77
14192	O	HOH	X	746	42.653	29.458	71.470	1.00	22.38
14195	O	HOH	X	747	7.357	39.493	72.501	1.00	26.00
14198	O	HOH	X	748	8.168	40.692	68.191	1.00	24.98
14201	O	HOH	X	749	4.964	40.635	69.073	1.00	28.88
14204	O	HOH	X	750	13.772	33.482	45.348	1.00	27.82
14207	O	HOH	X	751	25.374	31.261	19.992	1.00	23.73
14210	O	HOH	X	752	21.226	29.765	18.764	1.00	26.07
14213	O	HOH	X	753	15.986	32.135	22.076	1.00	24.78
14216	O	HOH	X	754	19.263	29.936	20.408	1.00	26.06
14219	O	HOH	X	755	23.451	19.849	30.360	1.00	21.78
14222	O	HOH	X	756	34.200	29.874	27.826	1.00	28.13
14225	O	HOH	X	757	21.809	42.208	57.845	1.00	23.79
14228	O	HOH	X	758	17.448	40.187	55.912	1.00	20.20
14231	O	HOH	X	759	13.716	42.895	60.189	1.00	24.66
14234	O	HOH	X	760	14.045	49.867	60.803	1.00	25.65
14237	O	HOH	X	761	9.095	55.322	61.639	1.00	25.93
14240	O	HOH	X	762	37.080	13.569	34.728	1.00	34.70
14243	O	HOH	X	763	39.415	14.029	32.179	1.00	38.98
14246	O	HOH	X	764	40.689	12.113	33.046	1.00	22.53

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
14249	O	HOH	X	765	42.772	13.616	33.119	1.00	28.19
14252	O	HOH	X	766	44.040	12.976	35.371	1.00	25.74
14255	O	HOH	X	767	42.129	16.316	32.636	1.00	26.13
14258	O	HOH	X	768	38.491	36.919	28.582	1.00	23.63
14261	O	HOH	X	769	39.039	35.217	26.639	1.00	25.31
14264	O	HOH	X	770	33.881	38.944	24.308	1.00	29.37
14267	O	HOH	X	771	30.539	38.266	20.965	1.00	28.70
14270	O	HOH	X	772	33.227	36.312	24.509	1.00	25.82
14273	O	HOH	X	773	28.650	46.001	72.027	1.00	21.58
14276	O	HOH	X	774	46.881	54.312	55.770	1.00	26.26
14279	O	HOH	X	775	53.975	49.841	65.628	1.00	25.28
14282	O	HOH	X	776	54.851	45.263	60.605	1.00	32.37
14285	O	HOH	X	777	53.307	38.908	53.561	1.00	26.80
14288	O	HOH	X	778	60.481	28.976	41.467	1.00	26.94
14291	O	HOH	X	779	61.565	31.643	38.500	1.00	28.55
14294	O	HOH	X	780	57.399	26.810	38.424	1.00	29.20
14297	O	HOH	X	781	36.840	33.219	37.951	1.00	25.66
14300	O	HOH	X	782	10.305	34.123	56.170	1.00	27.61
14303	O	HOH	X	783	17.162	33.648	55.200	1.00	21.59

FIGURE 4

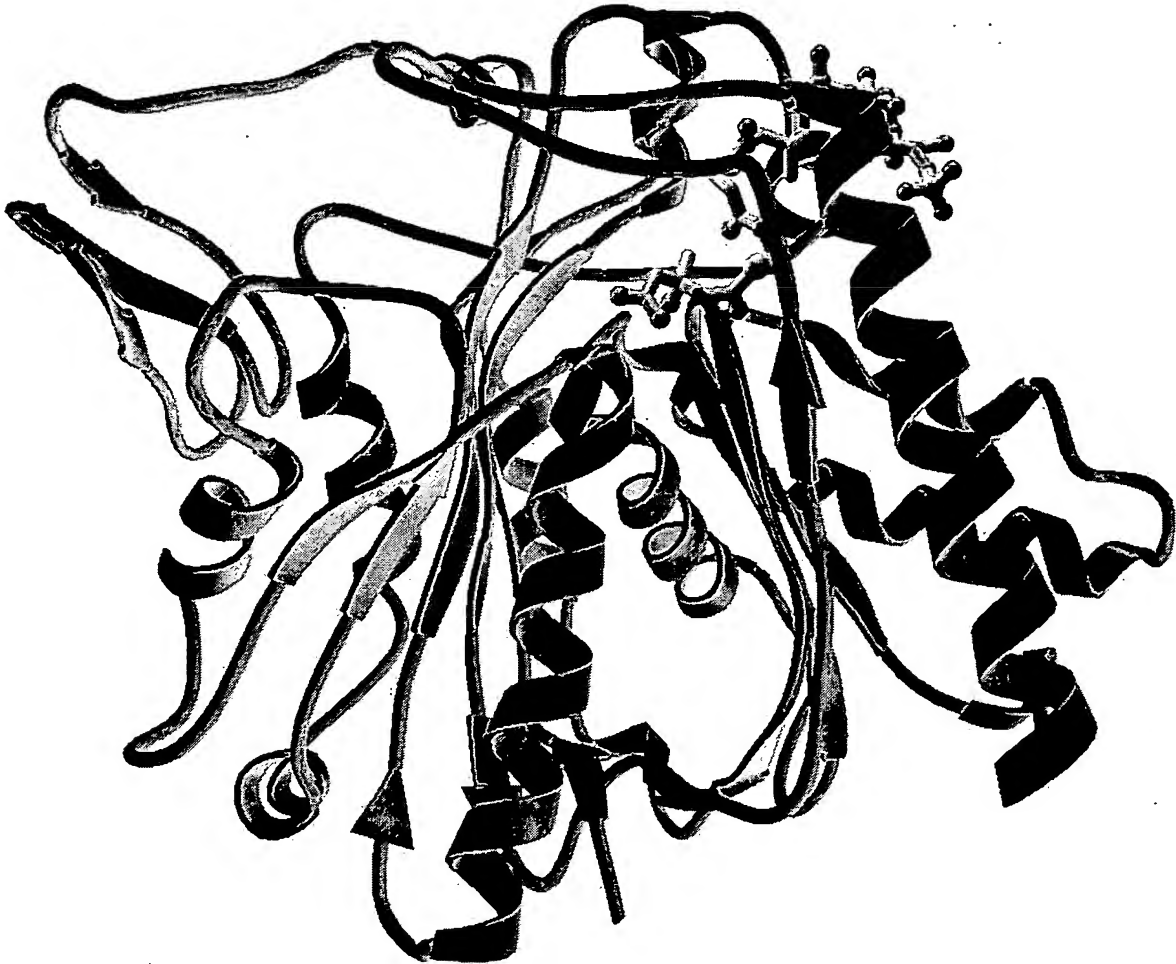


FIGURE 5

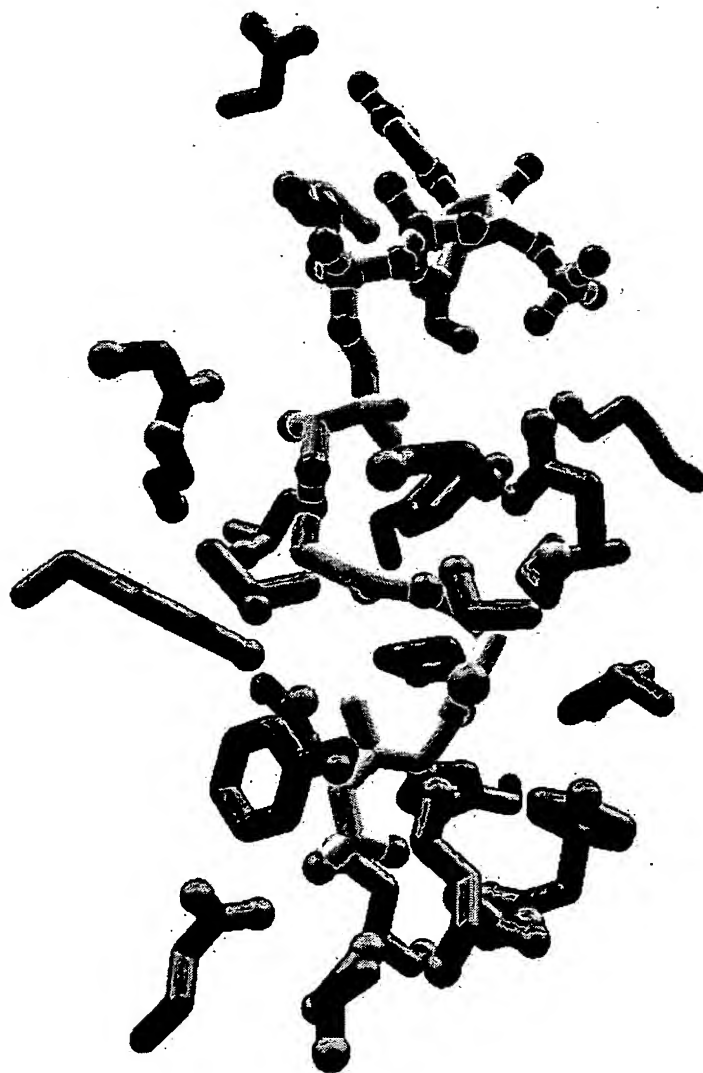


FIGURE 6

